

Electronic Supporting Information for

**Highly efficient Ti-catalyst for deoxygenative reduction of esters at ambient conditions:
experimental and mechanistic insights from DFT Study**

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TABLE OF CONTENTS

(S1) X-Ray crystallographic analyses:.....	1
(S2) NMR spectra for metal complexes:.....	3
(S3) Experimental details of ester hydroboration:.....	8
(S4) Characterization of ester hydroboration products:.....	8
(S5) NMR spectra of ester hydroboration products:.....	12
(S6) Control Experiments:.....	45
(S7) Kinetic analysis details:.....	51
(S8) Computational Method:.....	61
(S9) Discussion on D→→I Conversion: Key Conformational Changes in Ti–O _a CH(CH ₃)O _b CH ₃ Fragment :.....	61
(S10) Discussion on J→→O Conversion: Key Changes in Acetaldehyde Orientation Around the Ti Center :.....	63
(S11) Energy Table for Figure 3:.....	65
(S12) Energy Table for Figure S85:.....	66
(S13) Energy Table for Figure S86:.....	66
(S14) Cartesian Coordinates of the Optimized Structures.....	67
(S15) References:.....	109

(S1) X-Ray crystallographic analyses:

Single crystals of complexes **1** were grown from a concentrated solution of toluene in an argon-filled atmosphere at -35 °C. A crystal of suitable dimensions of complexes **1** was mounted on a CryoLoop (Hampton Research Corp.) with a layer of light mineral oil and placed in a nitrogen stream at 100 K. All measurements were made on a Rigaku Supernova X-calibur Eos CCD detector with graphite monochromatic Cu-K α (1.54184 Å) radiation. Crystal data and structure refinement parameters of complexes **1** are summarized in Table TS1. The structures were solved by direct methods (SIR2004)^[1] and refined on F^2 by full-matrix least-squares methods, using SHELXL-97.^[2] Non-hydrogen atoms were anisotropically refined. H-atoms were included in the refinement on calculated positions riding on their carrier atoms. The function minimized was $[\sum w(F_o^2 - F_c^2)^2]$ ($w = 1 / [\sigma^2(F_o^2) + (aP)^2 + bP]$), where $P = (\text{Max}(F_o^2, 0) + 2F_c^2) / 3$ with $\sigma^2(F_o^2)$ from counting statistics. The function $R1$ and $wR2$ were $(\sum ||F_o| - |F_c||) / \sum |F_o|$ and $[\sum w(F_o^2 - F_c^2)^2 / \sum (wF_o^4)]^{1/2}$, respectively. A special position disordered toluene molecule was found in the asymmetric unit. The attempts to model the toluene molecule were not successful as it was disordered over more than one position and the refinements were unstable in SHELXL. Contributions to scattering due to this toluene molecule were removed using the solvent mask instruction implemented in Olex2 crystal structure analysis software and squeeze data has been appended at CIF file. The unit cell contains a total of four toluene molecules, each has an area of 175 Å³ and the corresponding electron count was 50. The ORTEP-3 program was used to draw the molecules of **1**. Crystallographic data (excluding structure factors) for the structures reported in this paper have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication no. CCDC 2022197 (**1**). Copies of the data can be obtained free of charge on application to CCDC, 12 Union Road, Cambridge CB21EZ, UK (fax: + (44)1223-336-033; email: deposit@ccdc.cam.ac.uk).

Table S1. Crystallography table of metal complexes **1**.

Crystal Parameters	1
CCDC No.	2022197
Empirical formula	C ₃₀ H ₃₀ B ₂ Cl ₂ N ₂ P ₂ Ti
Formula weight	620.92
<i>T</i> (K)	100 K
λ (Å)	1.54184
Crystal system	Monoclinic
Space group	I2/a
<i>a</i> (Å)	18.7202(9)
<i>b</i> (Å)	10.1285(3)
<i>c</i> (Å)	35.068(4)
α (°)	90.00
β (°)	90.837(8)
γ (°)	90.00
<i>V</i> (Å ³)	6648.4(8)
<i>Z</i>	8
<i>D</i> _{calc} g cm ⁻³	1.241
μ (mm ⁻¹)	4.727
<i>F</i> (000)	2560.0
Theta range for data collection	9.088 to 141.698 deg
Limiting indices	-17 ≤ <i>h</i> ≤ 22, -12 ≤ <i>k</i> ≤ 6 -42 ≤ <i>l</i> ≤ 42
Reflections collected / unique	13610 / 6284 [R(int) = 0.0284]
Completeness to theta	99.8 %
Absorption correction	Multi-scan
Max. and min. transmission	1.000 and 0.980
Refinement method	Full-matrix least-squares on <i>F</i> ²
Data / restraints / parameters	6284/0/354
Goodness-of-fit on <i>F</i> ²	1.035
Final R indices [<i>I</i> > 2σ(<i>I</i>)]	R1 = 0.0372 wR2 = 0.1012

(S2) NMR spectra for metal complexes:

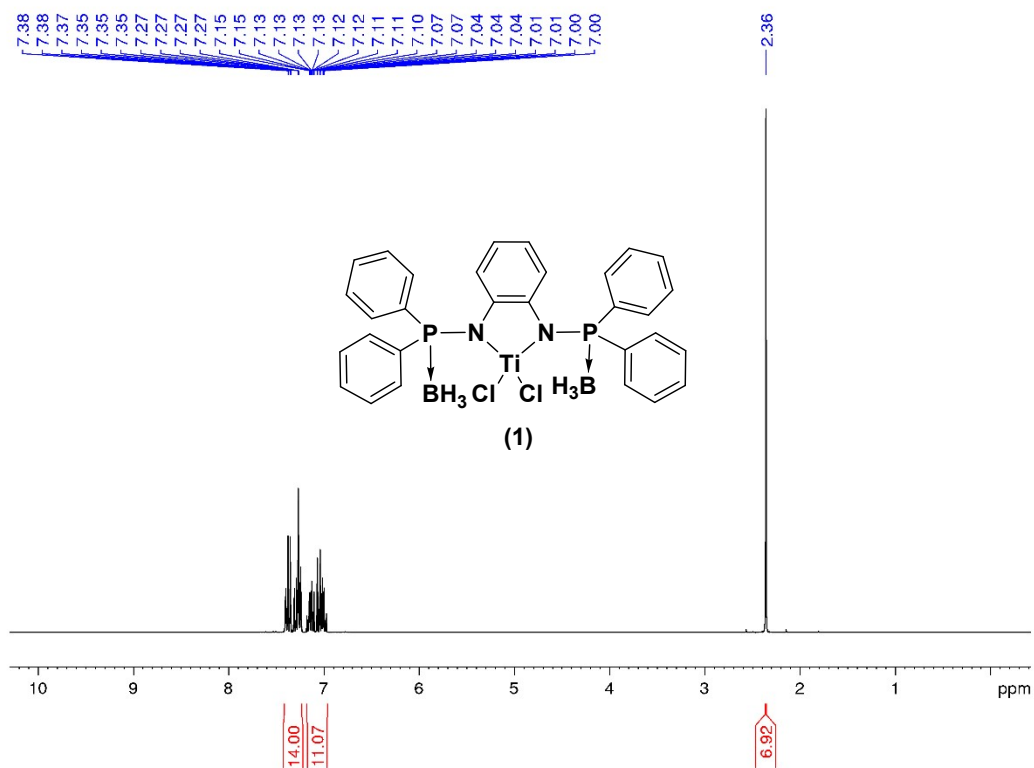


Figure S1. ¹H NMR spectrum (400 MHz, 25°C, C₆D₆) of compound 1.

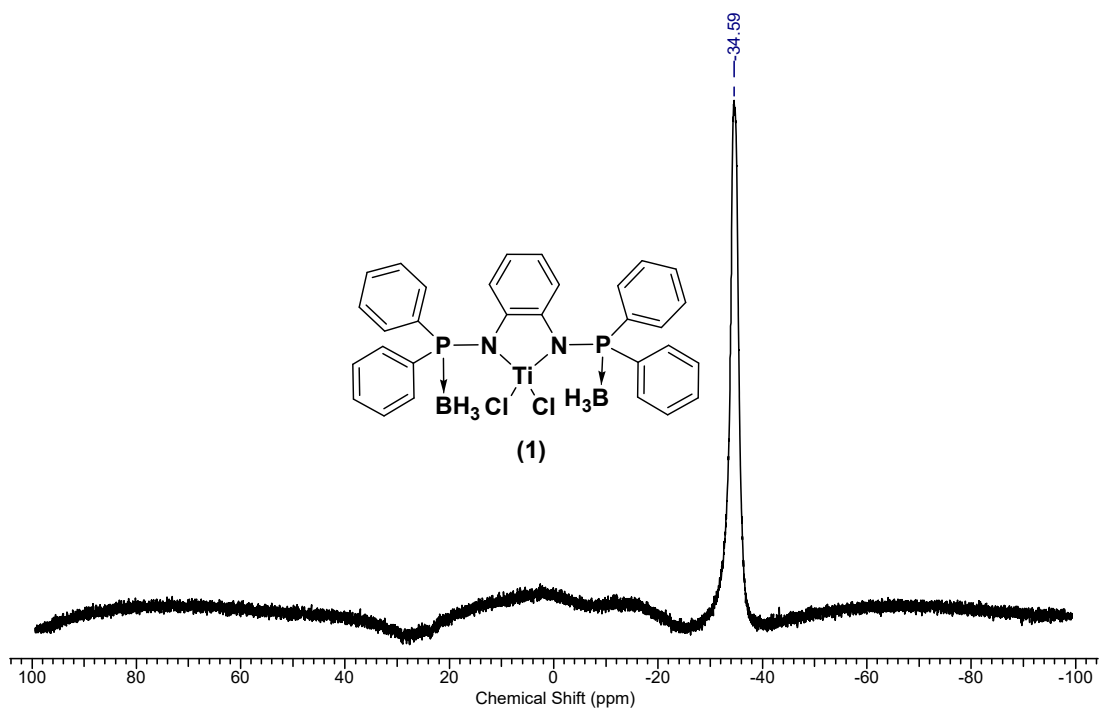


Figure S2. $^{11}\text{B}\{^1\text{H}\}$ NMR spectrum (128.4 MHz, 25°C, C_6D_6) of compound **1**.

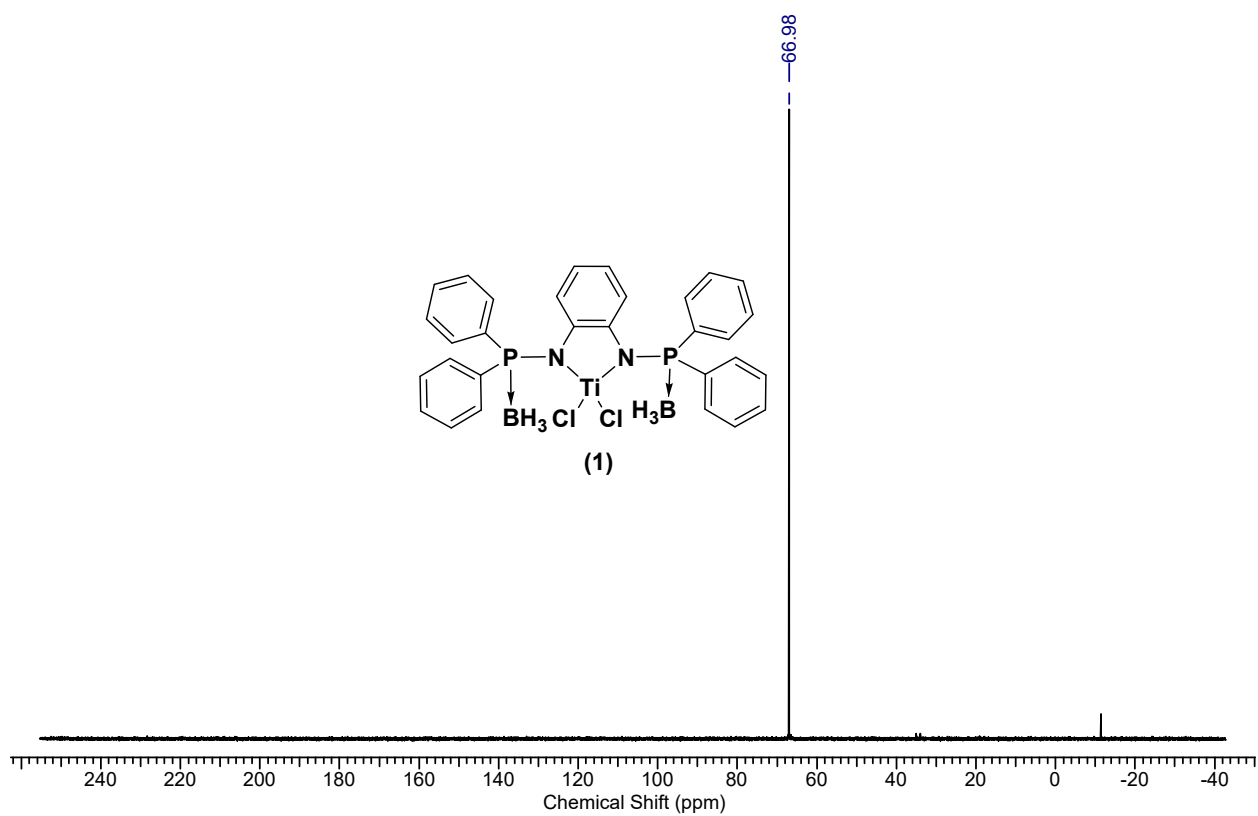


Figure S3. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum (161.9 MHz, 25°C, C_6D_6) of compound **1**.

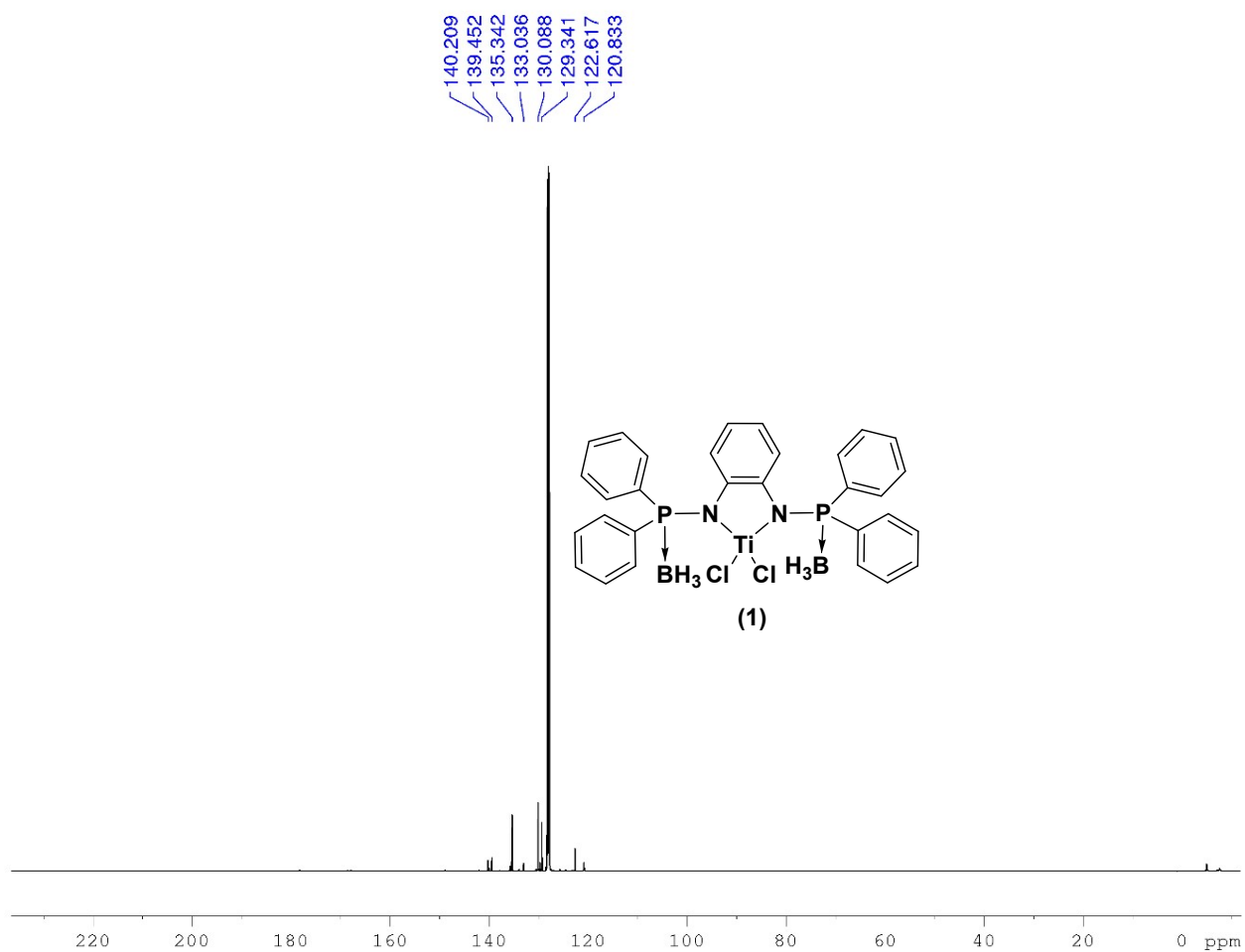


Figure S4. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (100 MHz, 25°C , C_6D_6) of compound **1**.

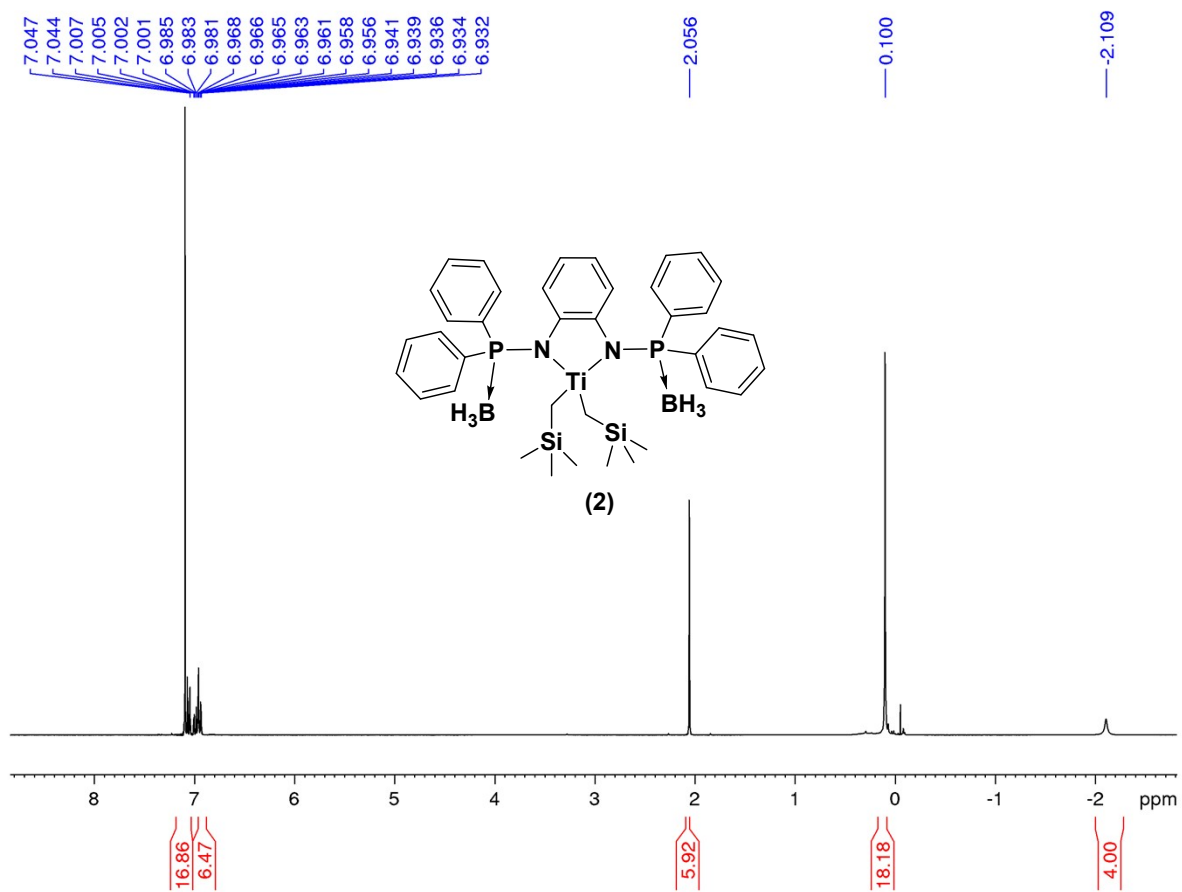


Figure S5: ¹H NMR spectrum (400 MHz, 25°C, C₆D₆) of compound **2**.

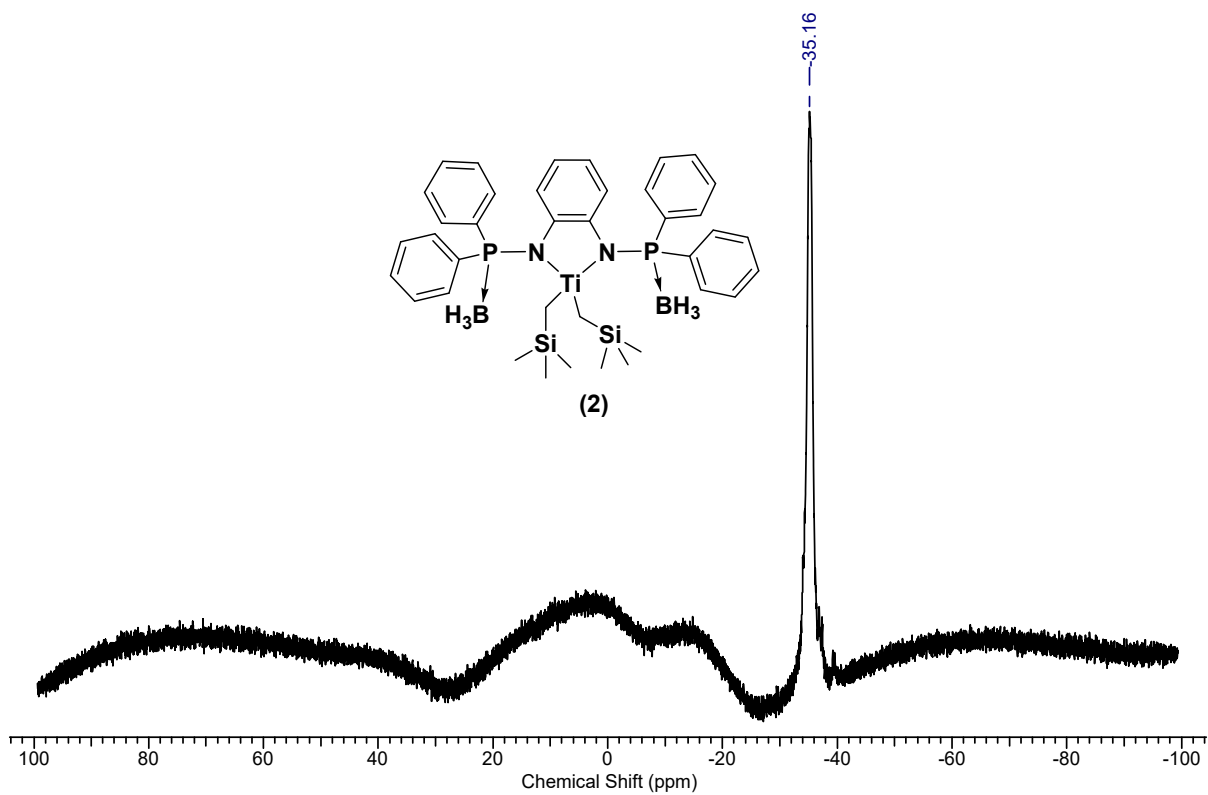


Figure S6: ¹¹B{¹H} NMR spectrum (128.4 MHz, 25°C, C₆D₆) of compound **2**.

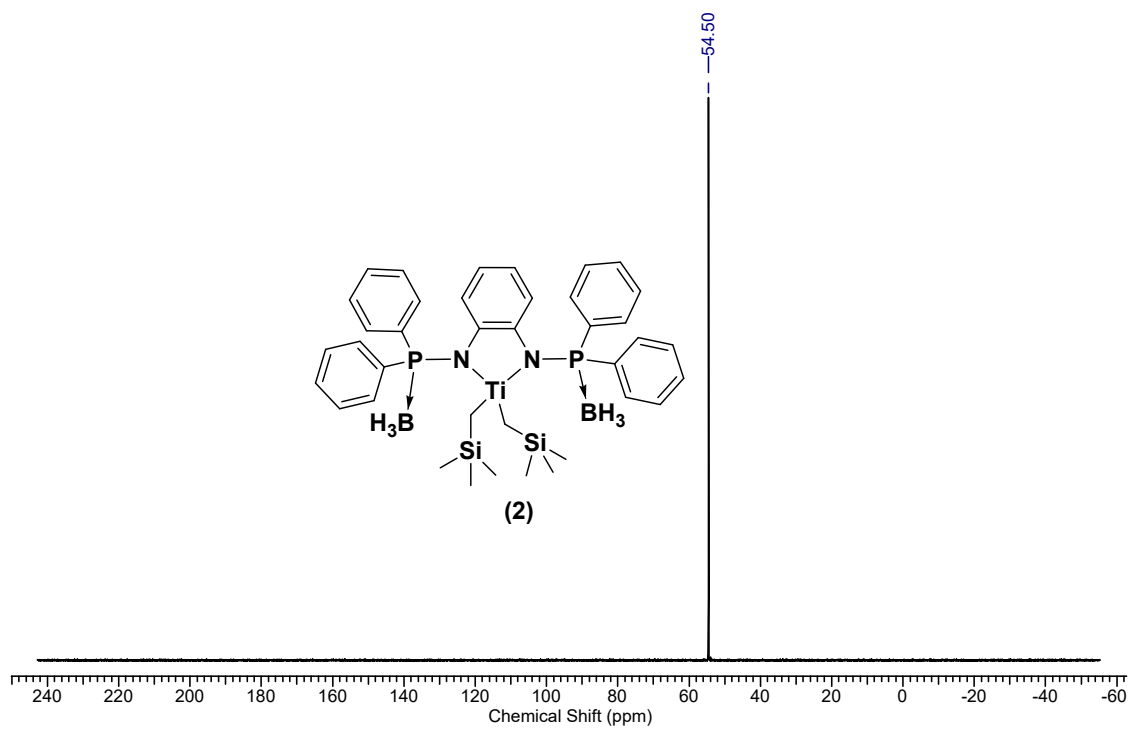


Figure S7: ³¹P{¹H} NMR spectrum (161.9 MHz, 25°C, C₆D₆) of compound **2**.

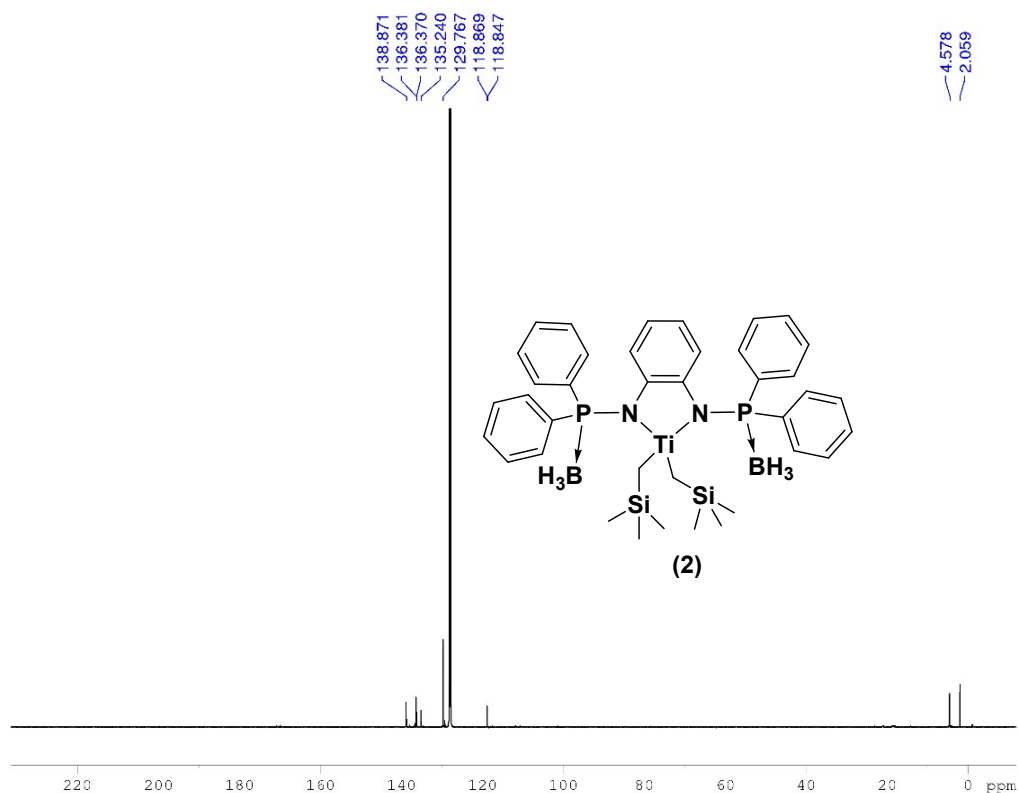


Figure S8. ¹³C{¹H} NMR spectrum (100 MHz, 25°C, C₆D₆) of compound **2**.

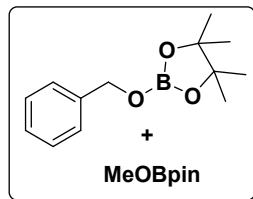
(S3) Experimental details of ester hydroboration:

General procedure for the hydroboration of esters

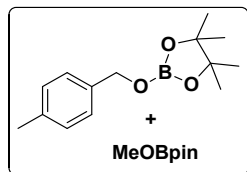
An oven-dried Schlenk flask was charged with 2 mol% catalyst **2** (7.25 mg, 0.01 mmol), required ester precursor (0.50 mmol, 1 equiv) and HBpin (1.0 mmol, 2.0 equiv). The reaction mixture was then placed at room temperature. In the case of solid esters, both the substrate were dissolved in benzene-*d*₆ (making total volume 1.0 mL). The progress of the reaction was monitored by ¹¹B and ¹H NMR where the product peaks were integrated with respect to the reactant peaks standardized with the –CH₃- the peak of the internal standard, HMB (8.0 mg, 0.05 mmol) which was normalized to 1.8. After the reaction was completed, the reaction mixture was evaporated under reduced pressure to obtain the desired compounds. Then the residue was washed with *n*-hexane (2 × 1 mL) to obtain **3a–3v**. Yields were calculated as an isolated yield basis.

(S4) Characterization of ester hydroboration products:

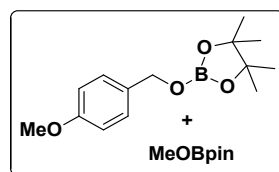
Characterization data for the products of ester reduction are given below. Previously reported products were characterized by ¹H, ¹¹B{¹H} and ¹³C{¹H} NMR.



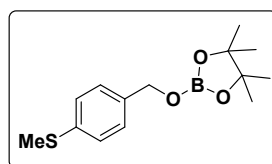
Yield (**3a**) (99%). ^1H NMR (400 MHz, C_6D_6): δ_{H} 7.99–7.96 (d, $J = 9.1$ Hz, 1H, ArH), 7.20–7.18 (m, 1H, ArH), 7.04–6.93 (m, 3H, ArH), 4.83 (s, 2H, CH_2), 0.94 (s, 12H, OBpin); $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, C_6D_6): δ_{C} 140.7, 133.5, 130.5, 127.7, 83.4, 67.6, 25.4 ppm; $^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, C_6D_6): δ_{B} 22.9 ppm, (**3b**): ^1H NMR (400 MHz, C_6D_6): δ_{H} 3.38 (s, 3H, BpinOCH₃), 0.92 (s, 12H, OBpin); $^{13}\text{C}\{^1\text{H}\}$ (100 MHz, C_6D_6): 83.2, 53.1, 25.4; $^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, C_6D_6): δ_{B} 22.9 ppm. NMR data are in accordance with the literature.^[3]



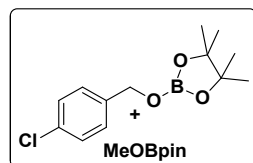
Yield (**3c**) (97%). ^1H NMR (400 MHz, C_6D_6): δ_{H} 7.24 (d, $J = 11.2$ Hz, 2H, ArH), 6.73 (d, $J = 11.2$ Hz, 2H, ArH), 4.91 (s, 2H, CH_2), 2.10 (s, 3H, ArCH₃), 1.04 (s, 12H, OBpin); $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, C_6D_6): δ_{C} 137.8, 137.6, 129.9, 127.9, 83.8, 67.6, 25.6, 21.8 ppm; $^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, C_6D_6): δ_{B} 22.9 ppm, (**3b**): ^1H NMR (400 MHz, C_6D_6): δ_{H} 3.28 (s, 3H, BpinOCH₃), 1.02 (s, 12H, OBpin); $^{13}\text{C}\{^1\text{H}\}$ (100 MHz, C_6D_6): 83.2, 53.1, 25.4 ppm; $^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, C_6D_6): δ_{B} 22.9 ppm. NMR data are in accordance with the literature.^[3]



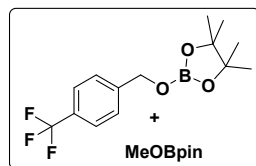
Yield (**3d**) (97%). ^1H NMR (400 MHz, C_6D_6): δ_{H} 7.25 (d, $J = 11.2$ Hz, 2H, ArH), 6.74 (d, $J = 11.2$ Hz, 2H, ArH), 4.90 (s, 2H, CH_2), 3.31 (s, 3H, OCH₃), 1.05 (s, 12H, OBpin); $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, C_6D_6): δ_{C} 160.3, 132.6, 129.5, 114.6, 83.3, 67.4, 55.5, 25.7 ppm; $^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, C_6D_6): δ_{B} 22.9 ppm, (**3b**): ^1H NMR (400 MHz, C_6D_6): δ_{H} 3.31 (s, 3H, BpinOCH₃), 1.04 (s, 12H, OBpin); $^{13}\text{C}\{^1\text{H}\}$ (100 MHz, C_6D_6): 83.2, 55.4, 25.4; $^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, C_6D_6): δ_{B} 22.9 ppm. NMR data are in accordance with the literature.^[3]



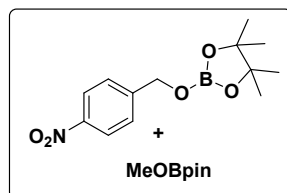
Yield (**3e**) (96%). ^1H NMR (400 MHz, CDCl_3): δ_{H} 7.14 (d, $J = 8.4$ Hz, 2H, ArH), 7.06 (d, $J = 8.1$ Hz, 2H, ArH), 4.08 (s, 2H, CH_2), 2.32 (s, 3H, CH₃), 1.09 (s, 12H, OBpin); $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3): δ_{C} 144.7, 128.9, 126.6, 123.9, 74.2, 51.1, 23.8, 13.7 ppm; $^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, CDCl_3): δ_{B} 22.7 ppm.



Yield (**3f**) (98%). ^1H NMR (400 MHz, C_6D_6): δ_{H} 6.91–6.87 (m, 1H, ArH), 6.73–6.68 (m, 2H, ArH), 6.81–6.76 (m, 1H, ArH), 4.63 (s, 2H, CH_2), 0.93 (s, 12H, OBpin); $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, C_6D_6): δ_{C} 143.4, 135.8, 131.2, 126.2, 84.2, 67.3, 25.9 ppm; $^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, C_6D_6): δ_{B} 22.97 ppm, (**3b**): ^1H NMR (400 MHz, C_6D_6): δ_{H} 3.39 (s, 3H, BpinOCH₃), 0.92 (s, 12H, OBpin); $^{13}\text{C}\{^1\text{H}\}$ (100 MHz, C_6D_6): 83.2, 55.4, 25.3; $^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, C_6D_6): δ_{B} 22.9 ppm. NMR data are in accordance with the literature.^[3]

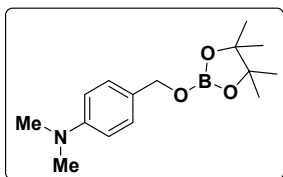


Yield (**3g**) (98%). ^1H NMR (400 MHz, C_6D_6): δ_{H} 7.31–7.28 (m, 2H, ArH), 7.09–7.07 (m, 2H, ArH), 4.78 (s, 2H, CH_2), 1.04 (s, 12H, OBpin); $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, C_6D_6): δ_{C} 144.5, 132.4, 127.5, 126.1, 83.6, 66.7, 25.4 ppm; $^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, CDCl_3): δ_{B} 22.9 ppm; $^{19}\text{F}\{^1\text{H}\}$ NMR (376.46 MHz, C_6D_6): δ_{F} -62.3 ppm, (**3b**): ^1H NMR (400 MHz, C_6D_6): δ_{H} 3.51 (s, 3H, BpinOCH₃), 1.00 (s, 12H, OBpin); $^{13}\text{C}\{^1\text{H}\}$ (100 MHz, C_6D_6): 83.2, 53.1, 25.3; $^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, C_6D_6): δ_{B} 22.9 ppm. NMR data are in accordance with the literature.^[3]

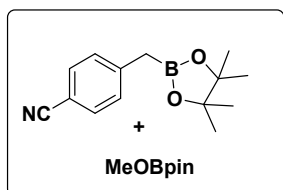


Yield (**3h**) (97%). ^1H NMR (400 MHz, C_6D_6): δ_{H} 7.79 (d, $J = 11.6$ Hz, 2H, ArH), 6.90 (d, $J = 11.6$ Hz, 2H, ArH), 4.69 (s, 2H, CH_2), 1.04 (s, 12H, OBpin); $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, C_6D_6): δ_{C} 148.2, 147.2, 127.4, 124.2, 83.7, 66.3, 25.4 ppm; $^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, C_6D_6): δ_{B} 22.9 ppm, (**3b**): ^1H NMR (400 MHz, C_6D_6): δ_{H} 3.51 (s, 3H, BpinOCH₃); $^{13}\text{C}\{^1\text{H}\}$ (100 MHz, C_6D_6): 83.2, 53.1, 25.3; $^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, C_6D_6): δ_{B} 22.9

ppm. The methyl peaks of -OBpin in ^1H NMR are overlapping in the region 1.04–1.02 ppm. NMR data are in accordance with the literature.^[3]

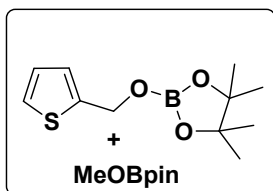


Yield (**3i**) (92%). ^1H NMR (400 MHz, CDCl_3): δ_{H} 7.29–7.27 (m, 1H, ArH), 7.11–7.08 (m, 1H, ArH), 6.52–6.47 (m, 2H, ArH), 4.01 (s, 2H, CH_2), 2.85–2.75 (s, 6H, $\text{N}(\text{CH}_3)_2$), 1.13–1.08 (s, 12H, OBpin); $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3): δ_{C} 131.7, 131.1, 110.5, 82.9, 82.6, 81.8, 80.1, 39.8, 24.6, 22.5 ppm; $^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, CDCl_3): δ_{B} 21.18 ppm. NMR data are in accordance with the literature.^[3]

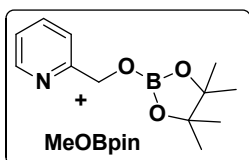


Yield (**3j**) (97%). ^1H NMR (400 MHz, CDCl_3): δ_{H} 7.00 (d, $J = 8.4$ Hz, 2H, ArH), 6.90 (d, $J = 8.4$ Hz, 2H, ArH), 4.67 (s, 2H, CH_2), 1.04 (s, 24H, OBpin); $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3): δ_{C} 145.5, 133.1, 128.0, 127.7, 84.1, 66.8, 25.9 ppm; $^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, CDCl_3): δ_{B} 22.20 ppm, (**3b**): ^1H NMR (400 MHz, C_6D_6): δ_{H} 3.50 (s, 3H, BpinOCH₃), 1.02 (s, 12H, OBpin); $^{13}\text{C}\{^1\text{H}\}$ (100 MHz, C_6D_6): 83.5, 53.4, 25.6; $^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, C_6D_6): δ_{B} 22.9 ppm. NMR data are in accordance with the

literature.^[3]

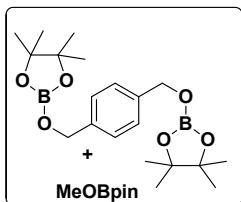


Yield (**3k**) (96%). ^1H NMR (400 MHz, C_6D_6): δ_{H} 6.87–6.82 (m, 2H, ArH), 6.66–6.65 (m, 1H, ArH), 4.99 (s, 2H, CH_2), 1.04 (s, 12H, OBpin); $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, C_6D_6): δ_{C} 143.4, 127.4, 126.7, 126.3, 83.5, 62.5, 25.6 ppm; $^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, C_6D_6): δ_{B} 22.95 ppm, (**3b**): ^1H NMR (400 MHz, C_6D_6): δ_{H} 3.49 (s, 3H, BpinOCH₃), 1.02 (s, 12H, OBpin); $^{13}\text{C}\{^1\text{H}\}$ (100 MHz, C_6D_6): 83.2, 53.0, 25.4; $^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, C_6D_6): δ_{B} 22.9 ppm. NMR data are in accordance with the literature.^[3]

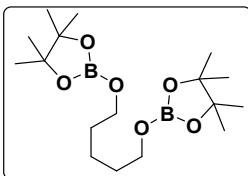


Yield (**3l**) (95%). ^1H NMR (400 MHz, CDCl_3): δ_{H} 8.67–8.45 (m, 2H, ArH), 7.33–7.31 (m, 1H, ArH), 6.71–6.70 (m, 1H, ArH), 4.72 (s, 2H, CH_2), 1.08–1.05 (s, 12H, OBpin); $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3): δ_{C} 150.0, 135.6, 134.9, 132.4, 123.9, 83.6, 65.3, 25.8; $^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, CDCl_3): δ_{B} 21.8 ppm, (**3b**): ^1H NMR (400 MHz, C_6D_6): δ_{H} 3.20 (s, 3H, BpinOCH₃), 1.02 (s, 12H, OBpin); $^{13}\text{C}\{^1\text{H}\}$ (100 MHz, C_6D_6): 83.2, 53.0, 25.4; $^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, C_6D_6): δ_{B} 22.9 ppm. NMR data are in accordance with the literature.^[3]

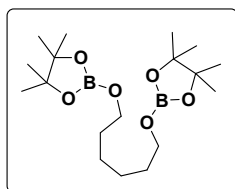
53.0, 25.4; $^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, C_6D_6): δ_{B} 22.9 ppm. NMR data are in accordance with the literature.^[3]



Yield (**3m**) (94%). ^1H NMR (400 MHz, CDCl_3): δ_{H} 7.24 (s, 4H, ArH), 4.90 (s, 4H, CH_2), 1.04 (s, 24H, OBpin); $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3): δ_{C} 138.8, 126.8, 82.4, 66.4, 24.5 ppm; $^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, CDCl_3): δ_{B} 22.49 ppm, (**3b**): ^1H NMR (400 MHz, C_6D_6): δ_{H} 3.49 (s, 3H, BpinOCH₃), 1.01 (s, 12H, OBpin); $^{13}\text{C}\{^1\text{H}\}$ (100 MHz, C_6D_6): 82.2, 52.0, 24.4; $^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, C_6D_6): δ_{B} 22.9 ppm. NMR data are in accordance with the literature.^[3]

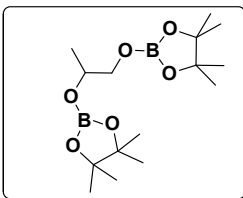


Yield (**3n**) (97%). ^1H NMR (400 MHz, CDCl_3): δ_{H} 3.54–3.50 (m, 4H, CH_2), 1.52–1.45 (m, 2H, CH_2), 1.38–1.35 (m, 2H, CH_2), 1.14 (s, 24H, OBpin); $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3): δ_{C} 129.4, 75.0, 67.7, 62.0, 38.8, 32.0, 29.6, 25.4, 24.4 ppm; $^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, CDCl_3): δ_{B} 22.09 ppm. NMR data are in accordance with the literature.^[3]



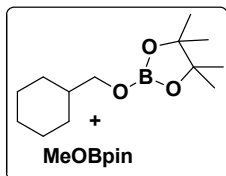
Yield (**3o**) (96%). ^1H NMR (400 MHz, C_6D_6): δ_{H} 3.90–3.85 (m, 4H, CH_2), 1.47–1.45 (m, 3H, CH_2), 1.25–1.20 (m, 3H, CH_2), 1.07 (s, 24H, OBpin); $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz,

C₆D₆): δ_C 83.0, 65.6, 32.6, 26.3, 25.4 ppm; $^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, C₆D₆): δ_B 22.76 ppm. NMR data are in accordance with the literature.^[3]

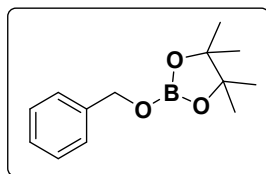


Yield (**3p**) (97%). ^1H NMR (400 MHz, C₆D₆): δ_H 4.54–4.49 (m, 1H, CH), 3.87–3.85 (m, 2H, CH₂), 1.11 (s, 24H, OBpin), 1.09–1.00 (m, 3H, CH₃); $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, C₆D₆): δ_C 83.1, 71.4, 70.2, 25.6, 21.2 ppm; $^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, C₆D₆): δ_B 22.80 ppm.

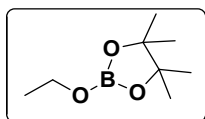
Hz, 2H, CH₂), 1.73–1.52 BpinOCy) ppm; ^{13}C NMR $^{11}\text{B}\{^1\text{H}\}$ NMR (96.3 MHz, (s, 3H, BpinOCH₃), 1.04 $^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, C₆D₆): δ_B 22.6 ppm. NMR data are in accordance with the literature.^[3]



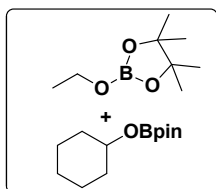
Yield (**3q**) (98%). ^1H NMR (300 MHz, C₆D₆): δ_H = 3.76 (d, J = 6.4 (m, 6H, BpinOCy), 1.07 (s, 12H, OC(CH₃)₂), 0.96–0.88 (m, 4H, (75.5 MHz, C₆D₆): δ_C = 83.2, 71.3, 40.5, 30.4, 27.5, 26.8, 25.4 ppm; C₆D₆): δ_B = 22.9 ppm, (**3b**): ^1H NMR (400 MHz, C₆D₆): δ_H 3.50 (s, 12H, OBpin); $^{13}\text{C}\{^1\text{H}\}$ (100 MHz, C₆D₆): 83.0, 53.0, 25.3;



Yield (**3a**) (98%). ^1H NMR (400 MHz, C₆D₆): δ_H 7.20–7.01 (d, J = 9.6 Hz, 2H, ArH), 6.99–6.93 (m, 3H, ArH), 4.83 (s, 2H, CH₂), 0.91 (s, 12H, OBpin); $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, C₆D₆): δ_C 140.7, 129.2, 128.2, 127.7, 83.3, 67.6, 25.3 ppm; $^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, C₆D₆): δ_B 23.1 ppm. NMR data are in accordance with the literature.^[3]

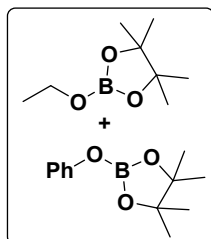


Yield (**3r**) (99%). ^1H NMR (400 MHz, C₆D₆): δ_H 3.92 (q, J = 7.0 Hz, 2H, CH₂CH₃), 1.12 (t, J = 8.1 Hz, 3H, CH₂CH₃), 1.06 (s, 12H, OBpin). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, C₆D₆): δ_C 83.0, 61.4, 25.4, 18.2 ppm. $^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, C₆D₆) δ_B 22.77 ppm. NMR data are in accordance with the literature.^[3]

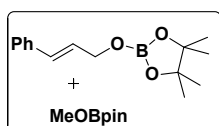


Yield (**3s**) (96%). ^1H NMR (400 MHz, C₆D₆): δ_H 4.13 – 4.04 (m, 1H, CHC₂H₅), 3.78 (q, 2H, CH₂CH₃), 1.79 - 1.48 (m, 10H, BpinOC₂H₅), 1.35 (t, 3H, CH₂CH₃), 1.07 (s, 24H, OBpin). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, C₆D₆): δ_C 83.0, 82.8, 73.3, 61.3, 35.4, 26.4, 25.4, 25.3, 24.7 ppm. $^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, C₆D₆) δ_B 22.7 ppm, (**3r**): ^1H NMR (400 MHz, C₆D₆): δ_H 3.92 (q, J = 7.0 Hz, 2H, CH₂CH₃), 1.12 (t, J = 8.1 Hz, 3H, CH₂CH₃), 1.06 (s, 12H, OBpin). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, C₆D₆): δ_C 83.0, 61.4, 25.4, 18.2 ppm. $^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, C₆D₆) δ_B

22.77 ppm. NMR data are in accordance with the literature.^[3]



Yield (**3r**) (9%). ^1H NMR (400 MHz, C₆D₆): δ_H 7.14 – 7.09 (m, 2H, Ar-H), 6.99 – 6.96 (m, 2H, Ar-H), 6.79 – 6.74 (m, 1H, Ar-H), 0.95 (s, 24H, OBpin). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, C₆D₆): δ_C 155.2, 130.4, 124.1, 120.9, 84.1, 25.5 ppm. $^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, C₆D₆) δ_B 22.9 ppm, (**3r**): ^1H NMR (400 MHz, C₆D₆): δ_H 3.81 (q, J = 7.0 Hz, 2H, CH₂CH₃), 1.02 (t, J = 8.2 Hz, 3H, CH₂CH₃), 0.95 (s, 12H, OBpin). $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, C₆D₆): δ_C 83.2, 61.5, 23.4 ppm. $^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, C₆D₆) δ_B 22.9 ppm. NMR data are in accordance with the literature.^[3]



Yield (**3u**) (96%): ^1H NMR (300 MHz, C₆D₆): δ_H = 7.19–7.01 (m, 5H, Ar-H), 6.60 (d, 1H, J = 15.9 Hz, CH), 6.19–6.14 (m, 1H, CH), 4.53 (d, 2H, J = 4.2 Hz, CH₂), 1.06 (s, 12H, OC(CH₃)₂) ppm; ^{13}C

$\{^1\text{H}\}$ NMR (75.5 MHz, C_6D_6): $\delta_{\text{C}} = 137.0, 131.4, 130.6, 128.5, 127.2, 126.5, 82.4, 65.2, 24.4$ ppm; ^{11}B $\{^1\text{H}\}$ NMR (96.3 MHz, C_6D_6): $\delta_{\text{B}} = 22.9$ ppm. (**3b**): ^1H NMR (400 MHz, C_6D_6): $\delta_{\text{H}} 3.50$ (s, 3H, BpinOCH_3), 1.03 (s, 12H, OBpin); $^{13}\text{C}\{^1\text{H}\}$ (100 MHz, C_6D_6): 82.2, 52.0, 24.1; $^{11}\text{B}\{^1\text{H}\}$ NMR (128 MHz, C_6D_6): $\delta_{\text{B}} 22.9$ ppm. NMR data are in accordance with the literature.^[3]

(S5) NMR spectra of ester hydroboration products:

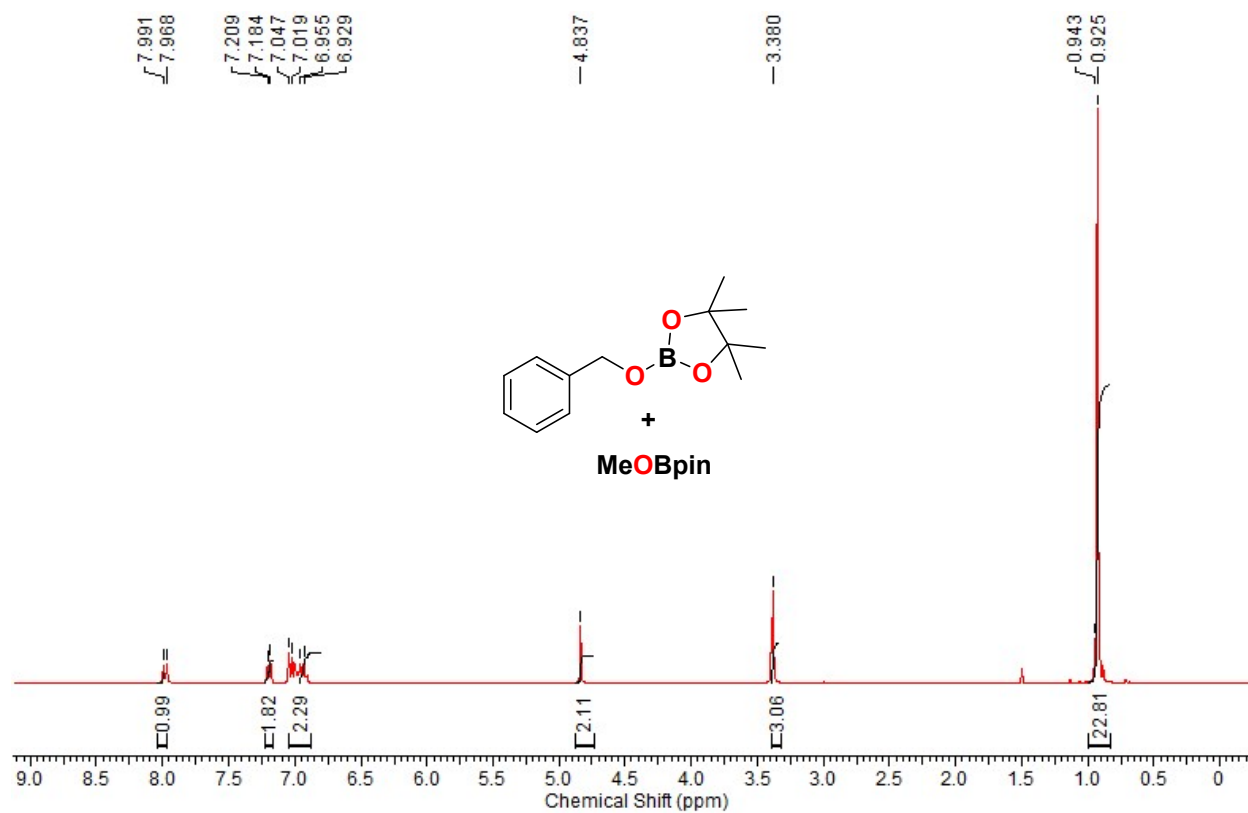


Figure S9. ^1H NMR spectrum (400 MHz, 25°C, C_6D_6) of compound **3a** and **3b**.

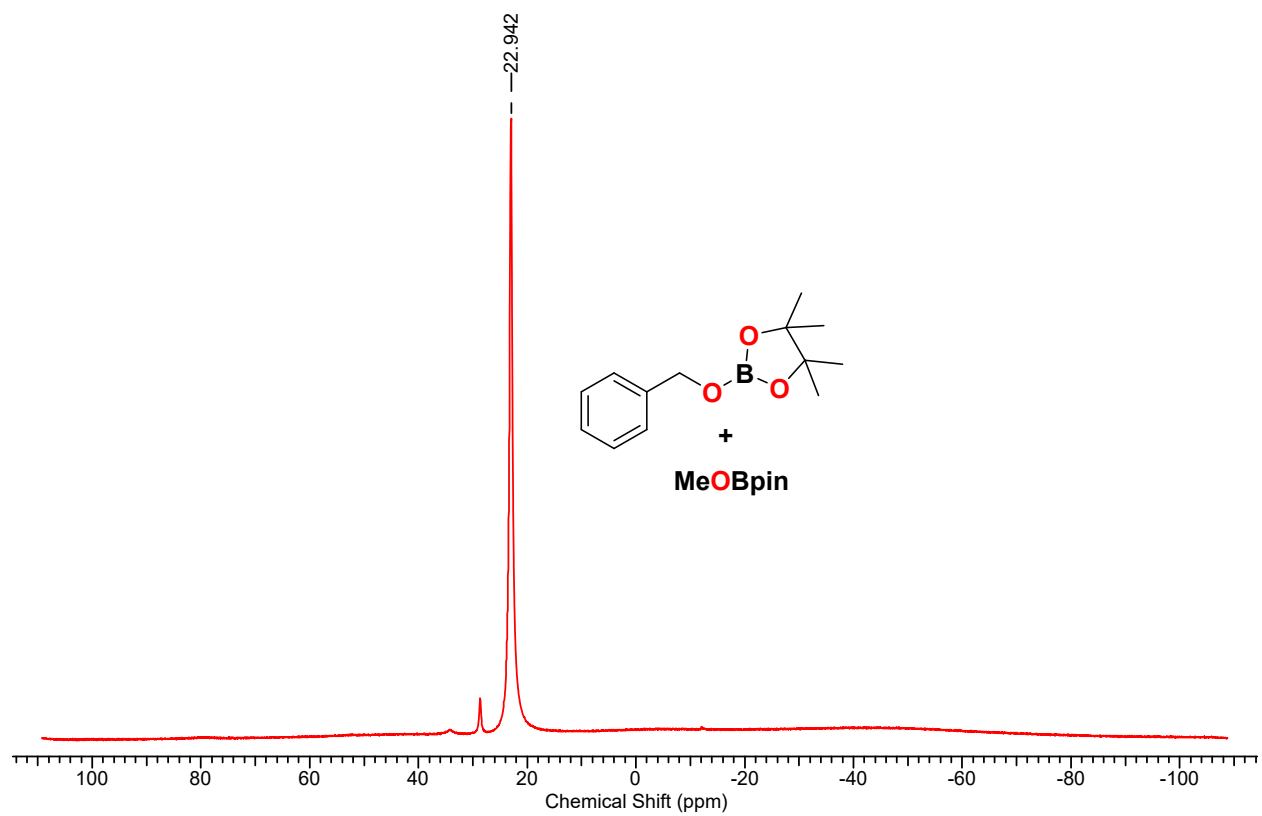


Figure S10. ^{11}B NMR spectrum (128.4 MHz, 25°C, C_6D_6) of compound **3a** and **3b**.

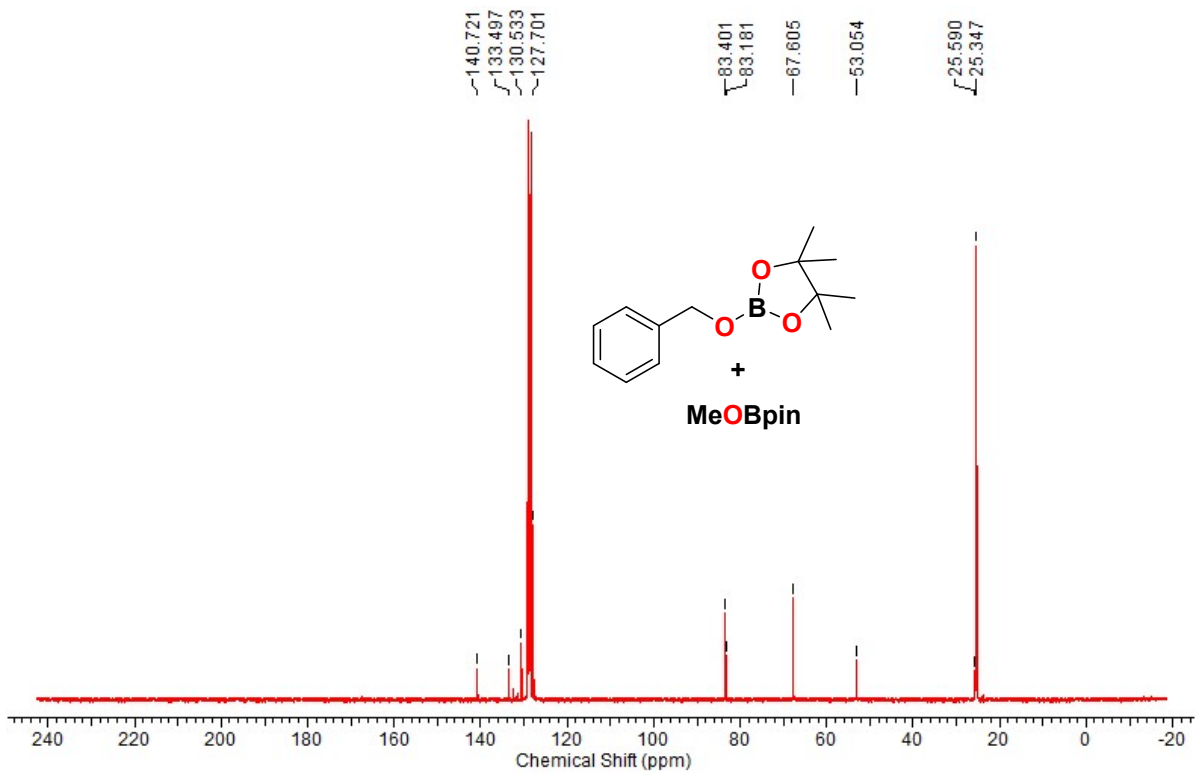


Figure S11: ^{13}C NMR spectrum (100 MHz, 25°C, C_6D_6) of compound **3a** and **3b**.

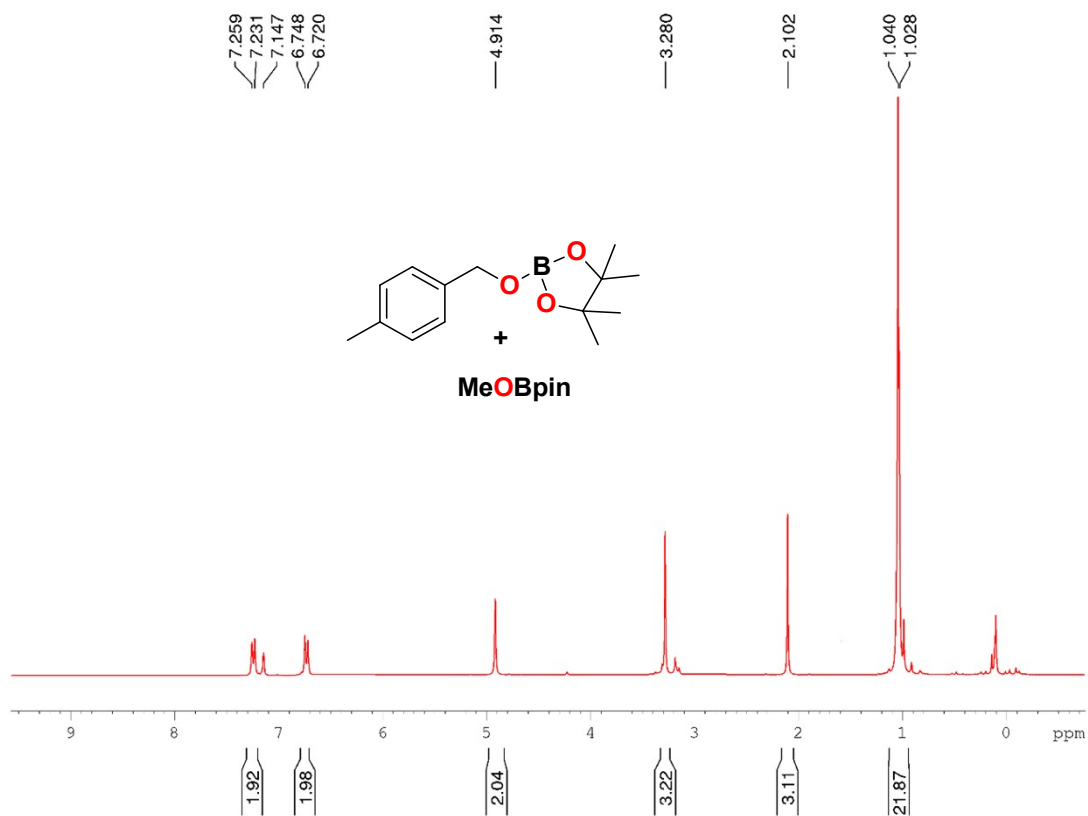


Figure S12: ^1H NMR spectrum (400 MHz, 25°C, C_6D_6) of compound **3c** and **3b**.

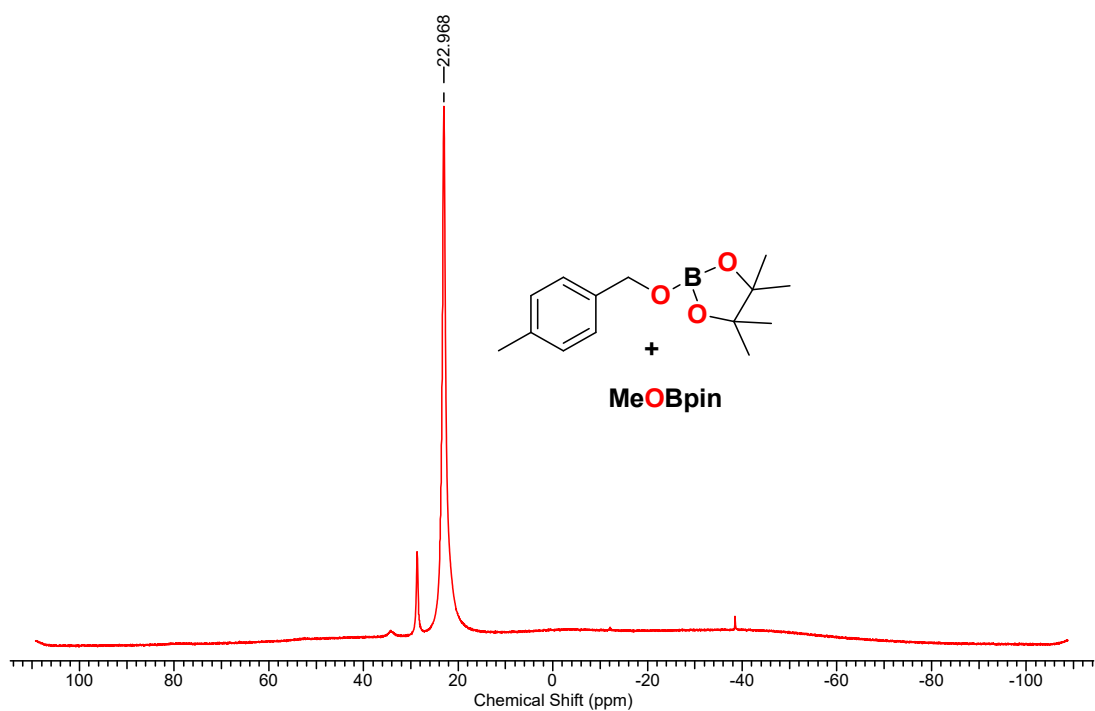


Figure S13. ^{11}B NMR spectrum (128.4 MHz, 25°C, C_6D_6) of compound **3c** and **3b**.

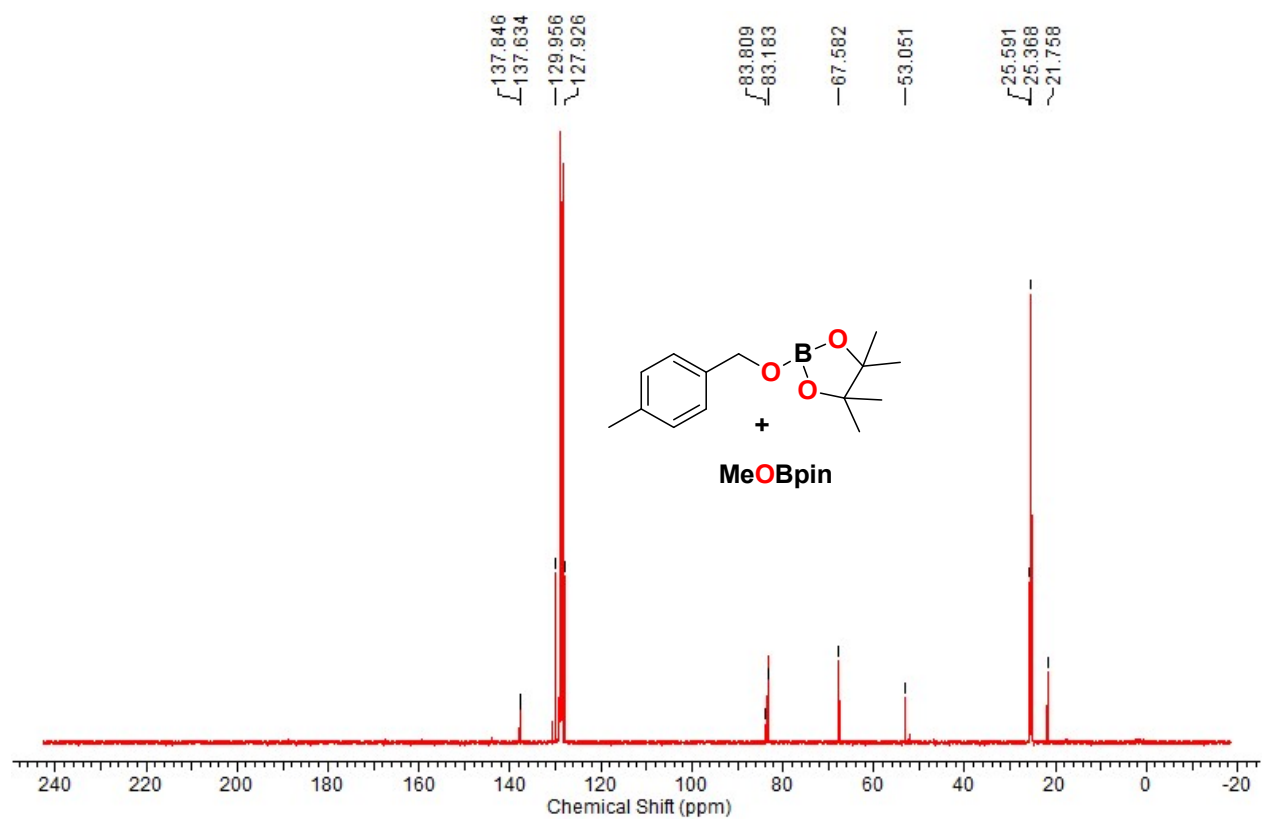


Figure S14. ^{13}C NMR spectrum (100 MHz, 25°C, C_6D_6) of compound **3c** and **3b**.

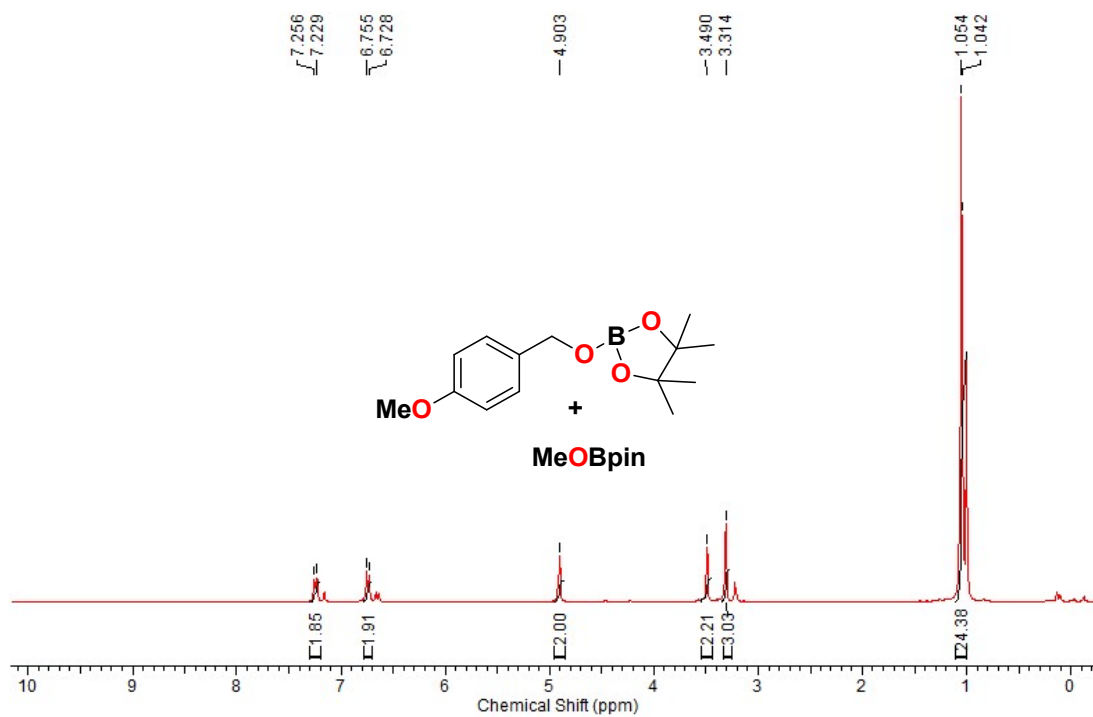


Figure S15. ^1H NMR spectrum (400 MHz, 25°C, C_6D_6) of compound **3d** and **3b**.

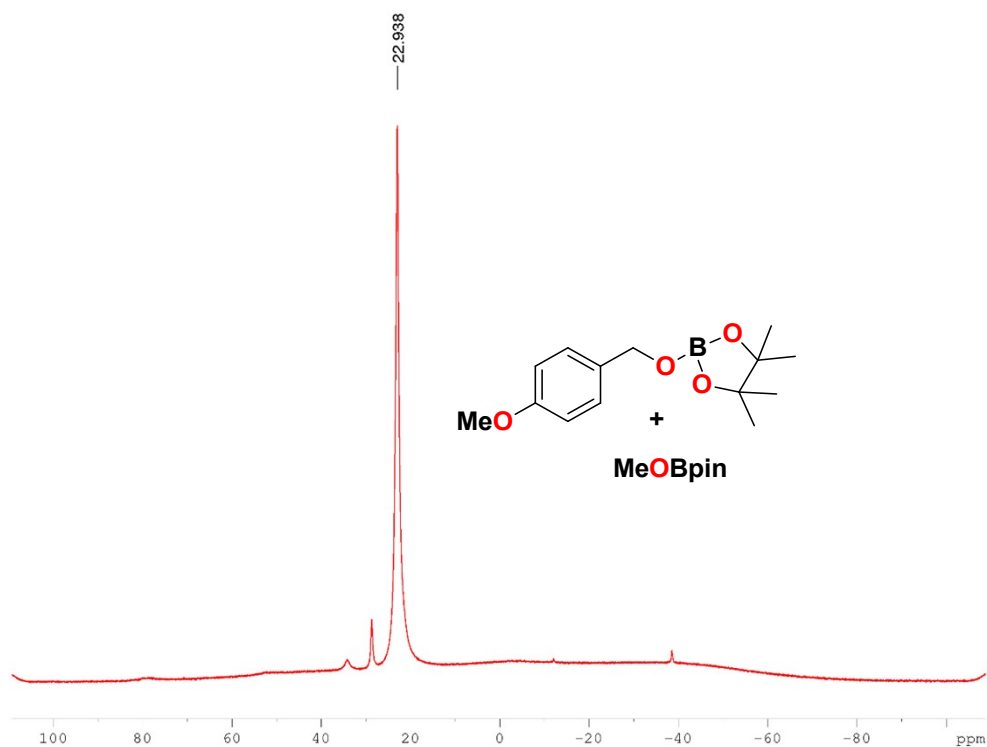


Figure S16. ^{13}B NMR spectrum (128.4 MHz, 25°C, C_6D_6) of compound **3d** and **3b**.

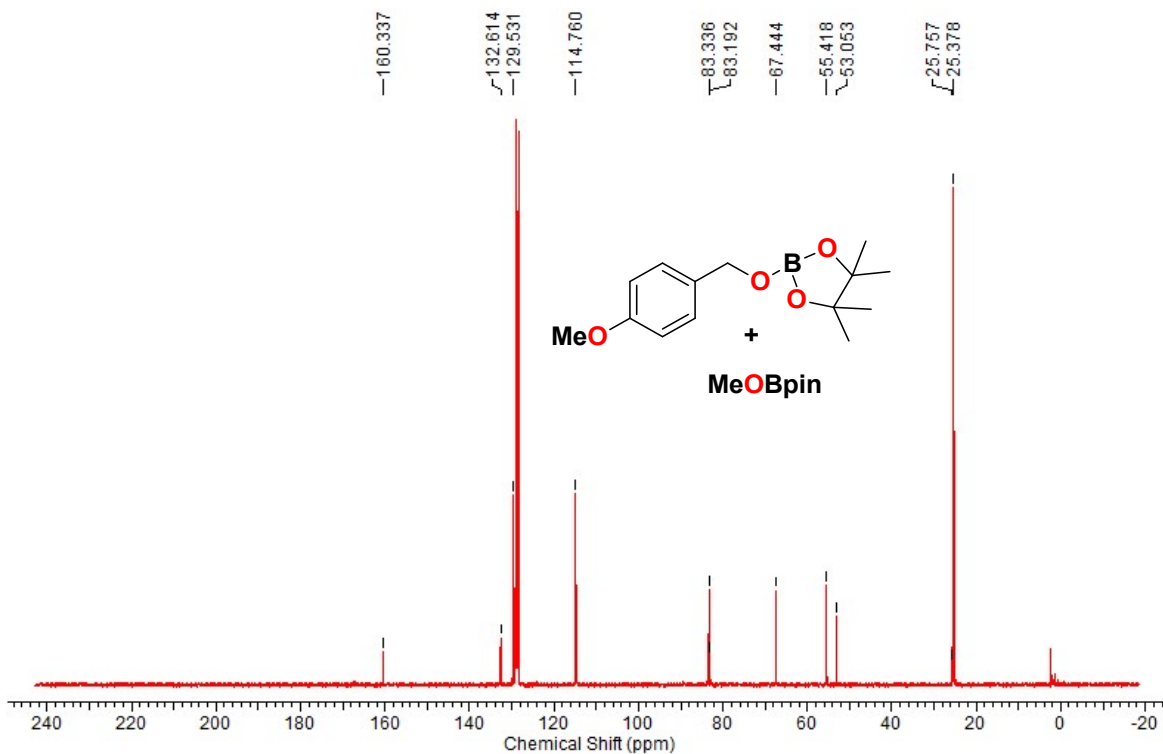


Figure S17. ^{13}C NMR spectrum (100 MHz, 25°C, C_6D_6) of compound **3d** and **3b**.

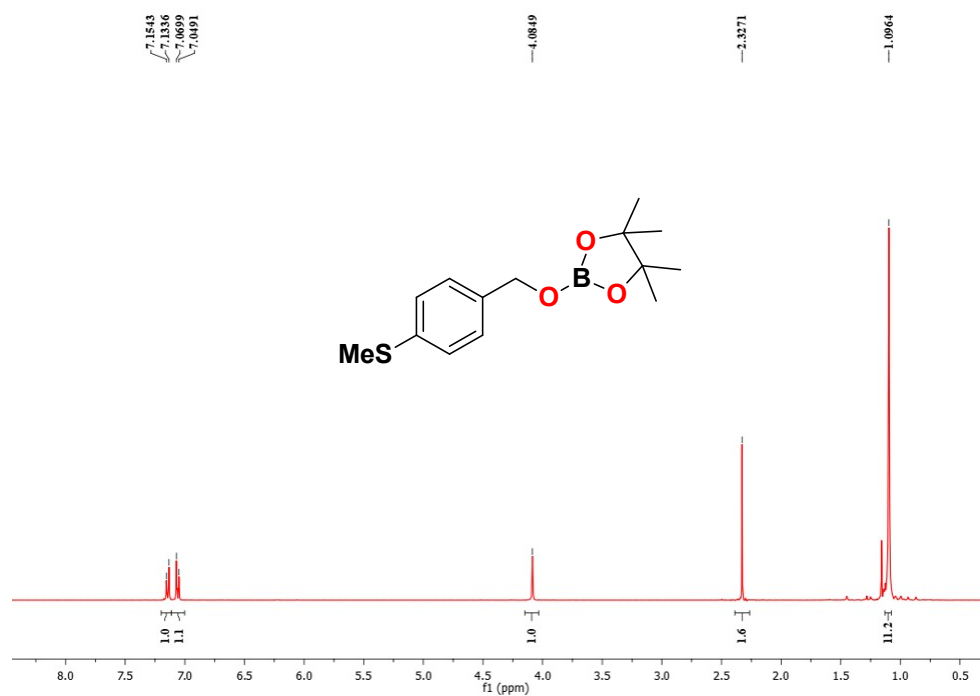


Figure S18. ^1H NMR spectrum (400 MHz, 25°C, CDCl_3) of compound **3e**.

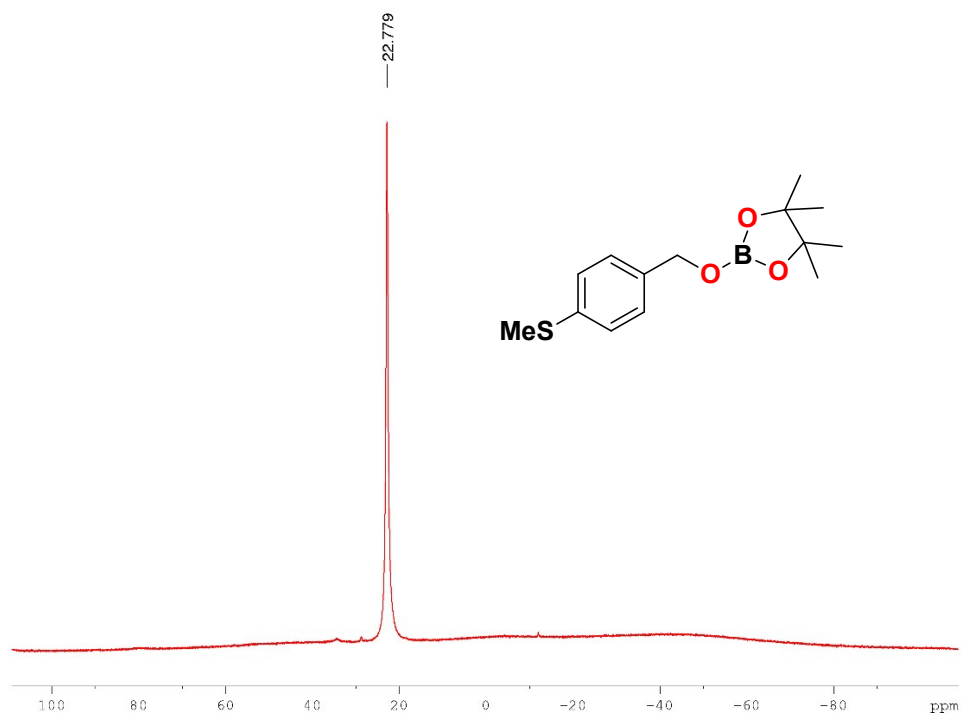


Figure S19. ^{11}B NMR spectrum (128.4 MHz, 25°C, CDCl_3) of **3e**.

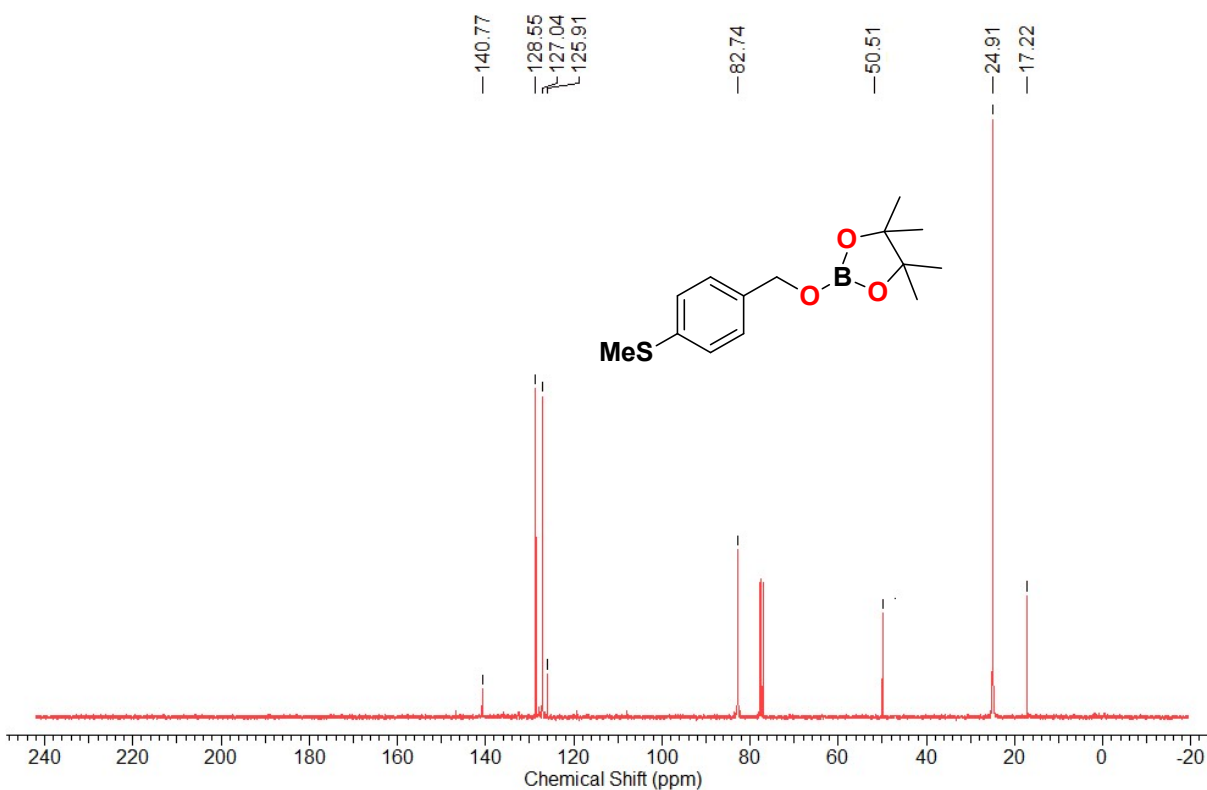


Figure S20. ^{13}C NMR spectrum (400 MHz, 25°C, CDCl_3) of compound **3e**.

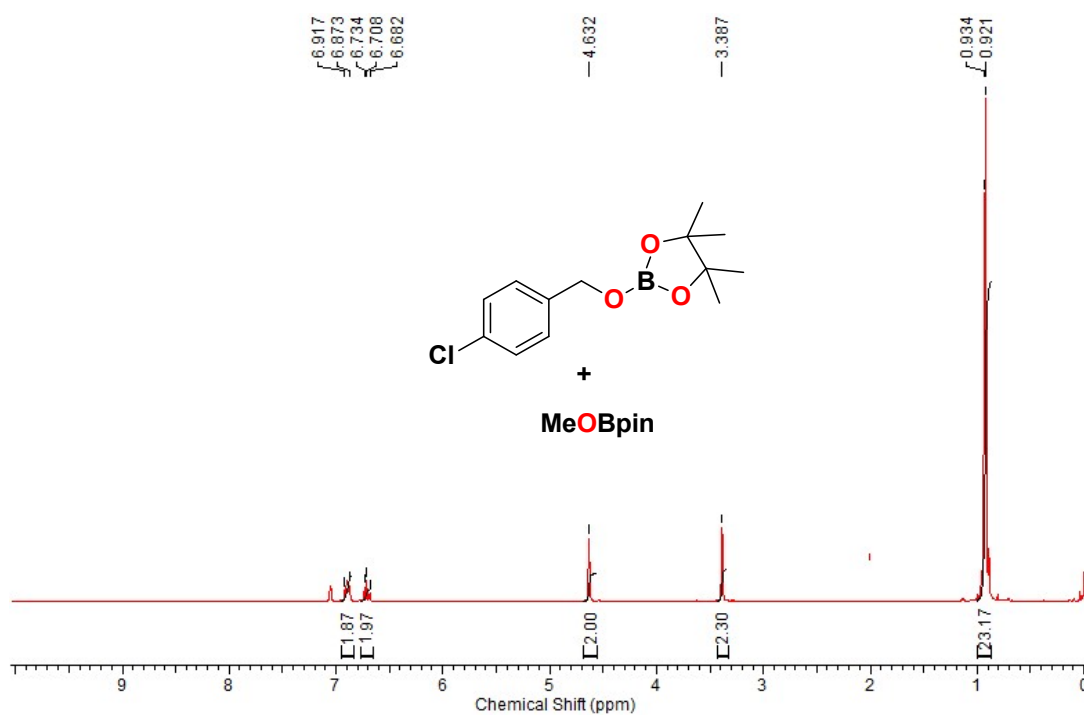


Figure S21. ^1H NMR spectrum (400 MHz, 25°C, C_6D_6) of compound **3f** and **3b**.

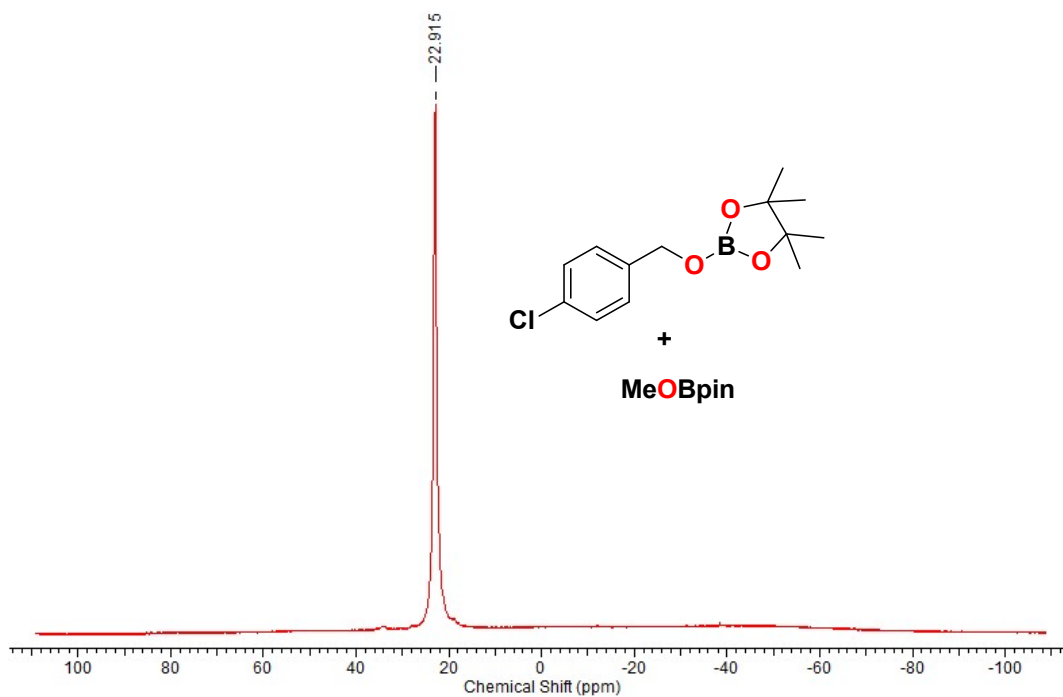


Figure S22. ^{11}B NMR spectrum (128.4 MHz, 25°C, C_6D_6) of compound **3f** and **3b**.

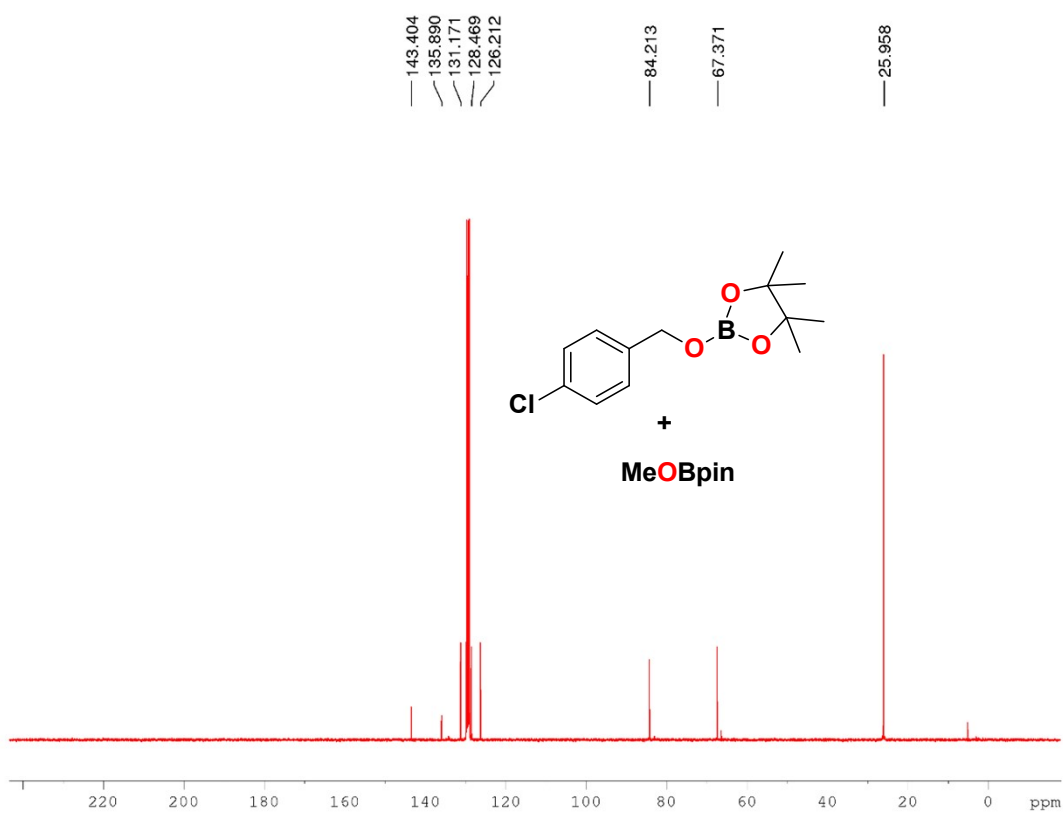


Figure S23. ^{13}C NMR spectrum (100 MHz, 25°C, C_6D_6) of compound **3f** and **3b**.

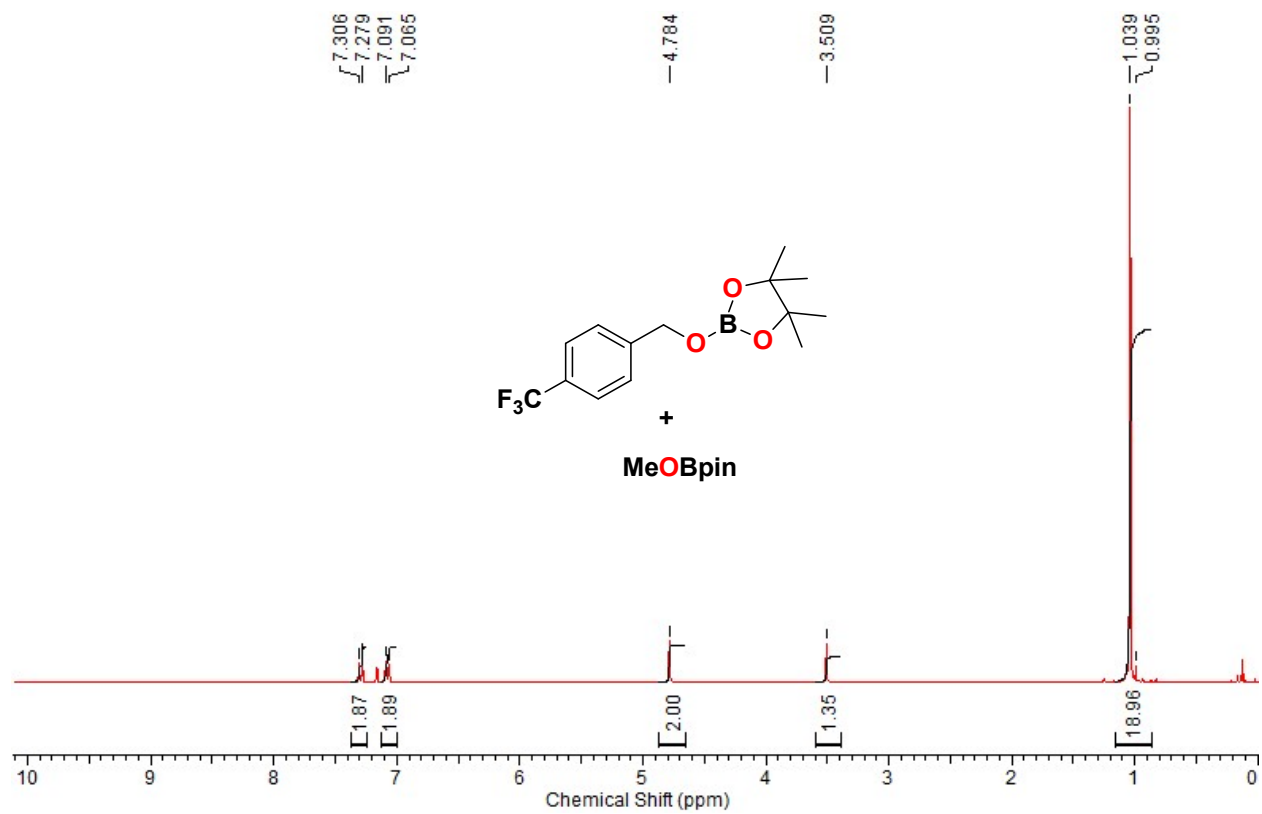


Figure 24. ¹H NMR spectrum (400 MHz, 25°C, C₆D₆) of compound **3g** and **3b**.

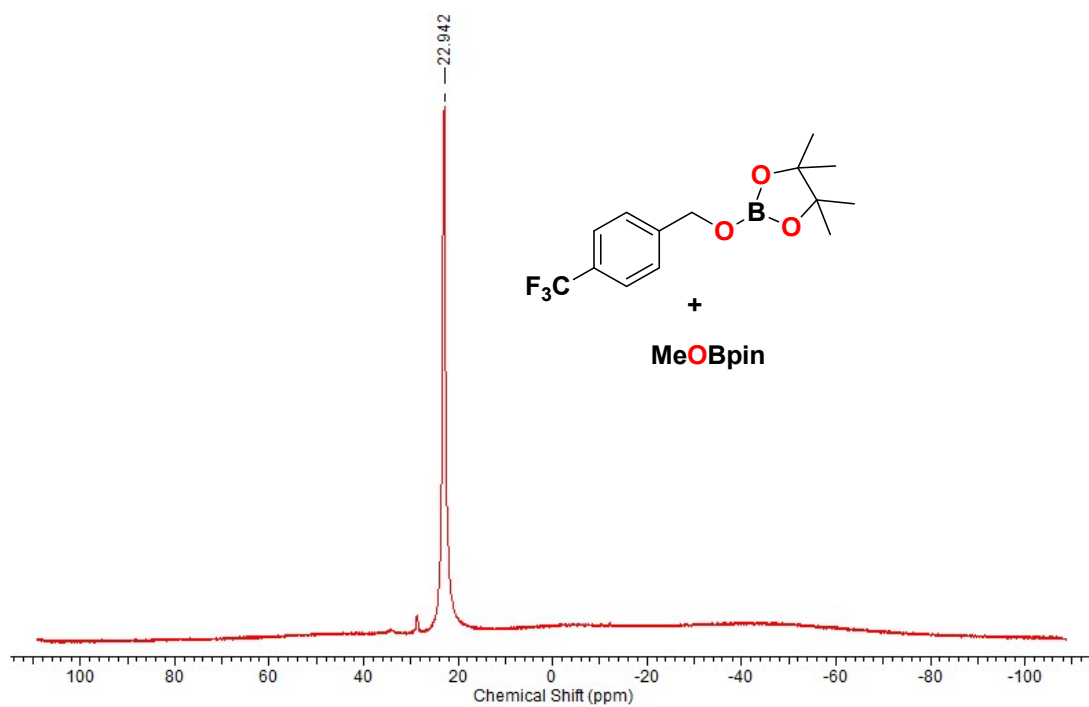


Figure S25. ¹¹B NMR spectrum (128.4 MHz, 25°C, C₆D₆) of compound **3g** and **3b**.

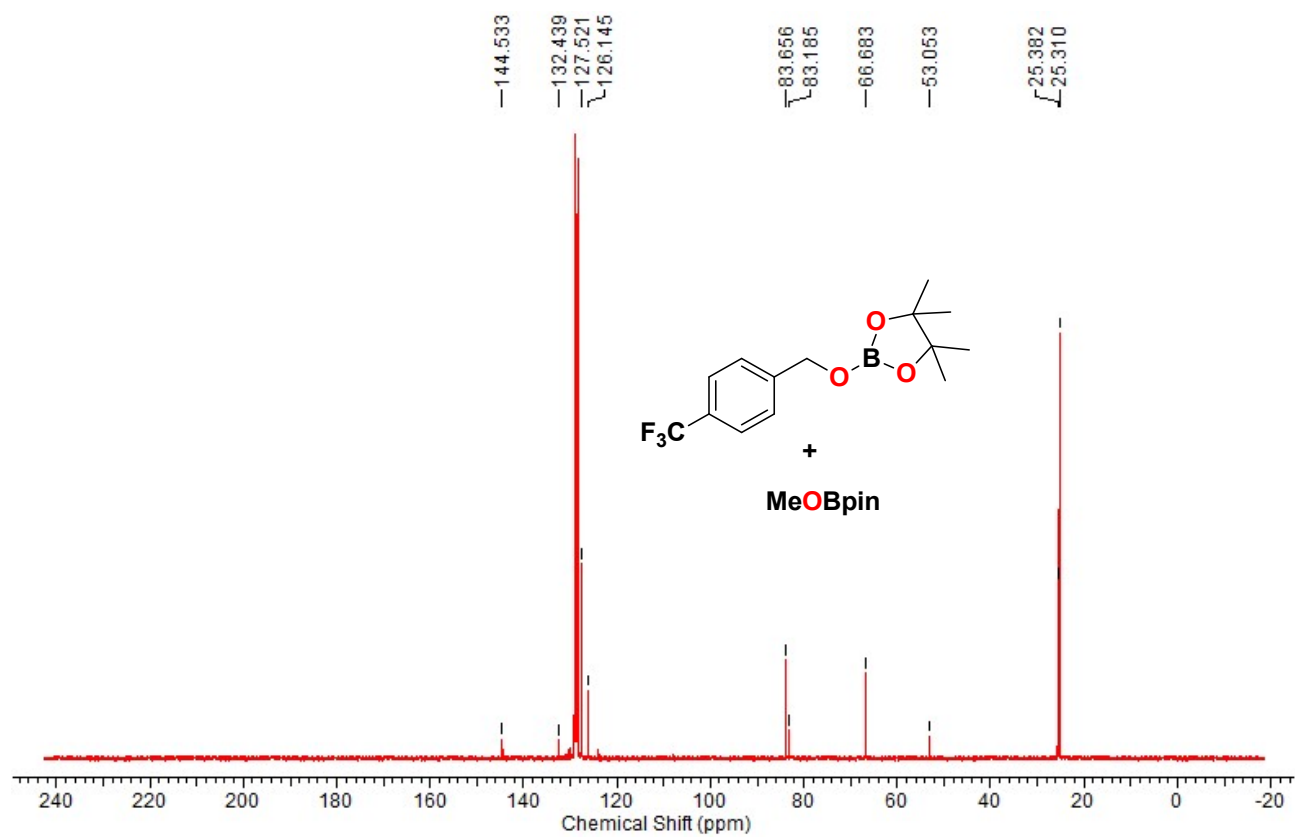
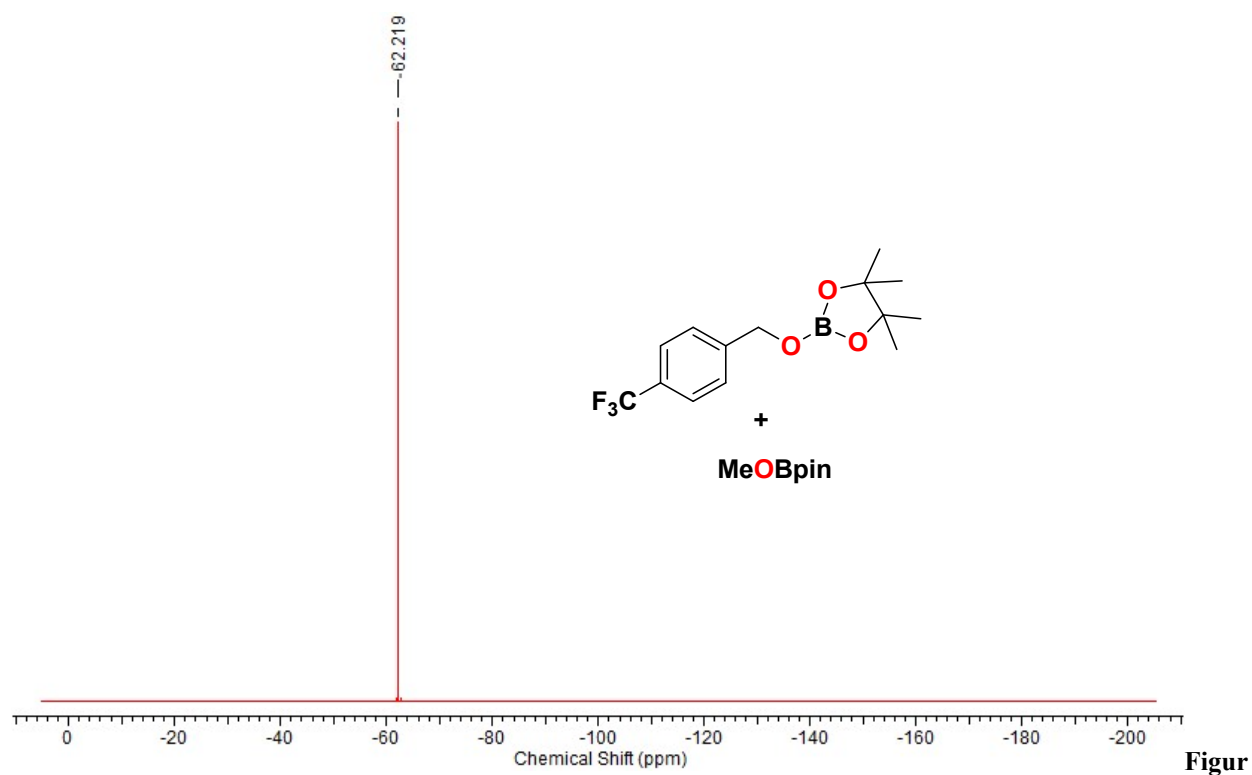


Figure S26. ^{13}C NMR spectrum (100 MHz, 25°C, C_6D_6) of compound **3g** and **3b**.



e S27. ^{19}F NMR spectrum (376.5 MHz, 25°C, C_6D_6) of compound **3g** and **3b**.

Figur

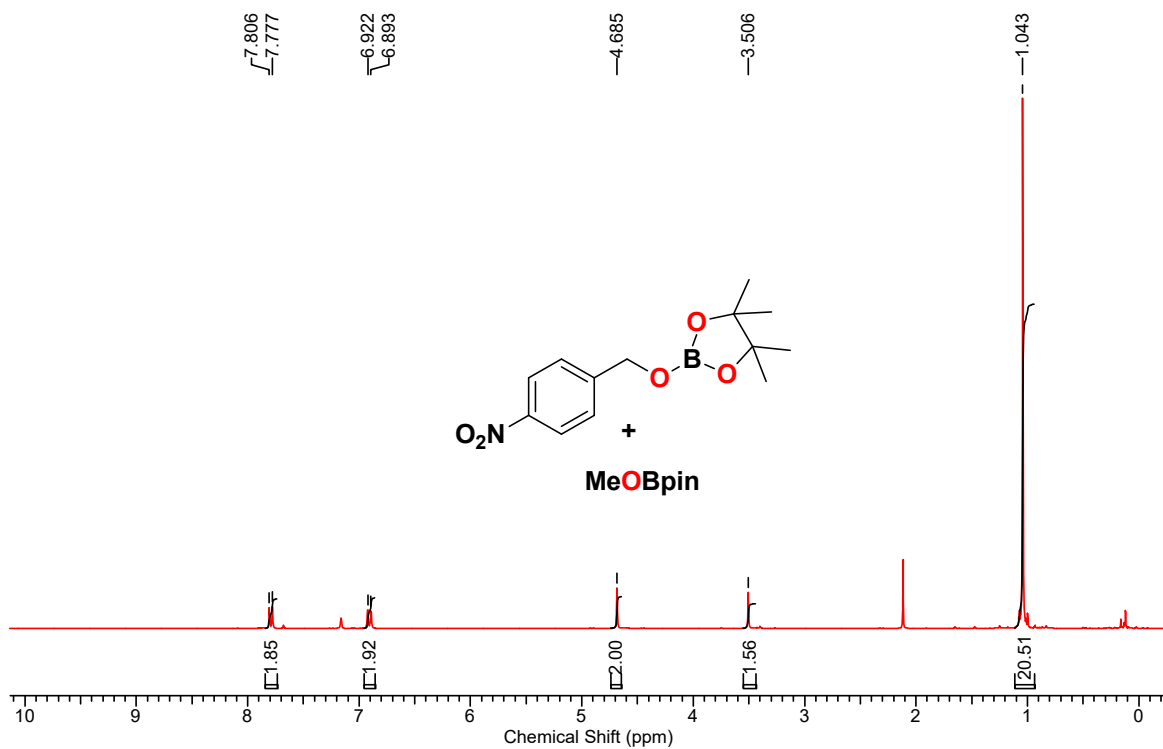


Figure S28. ^1H NMR spectrum (400 MHz, 25°C, C_6D_6) of compound **3h** and **3b**.

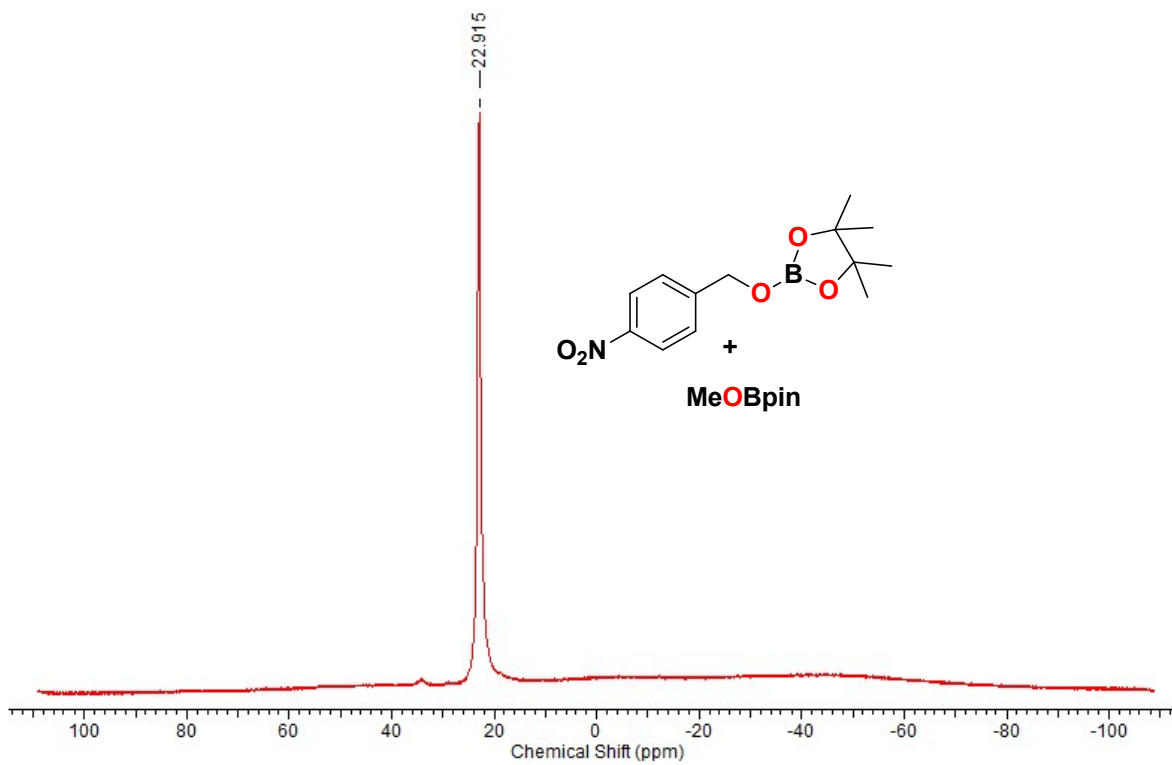
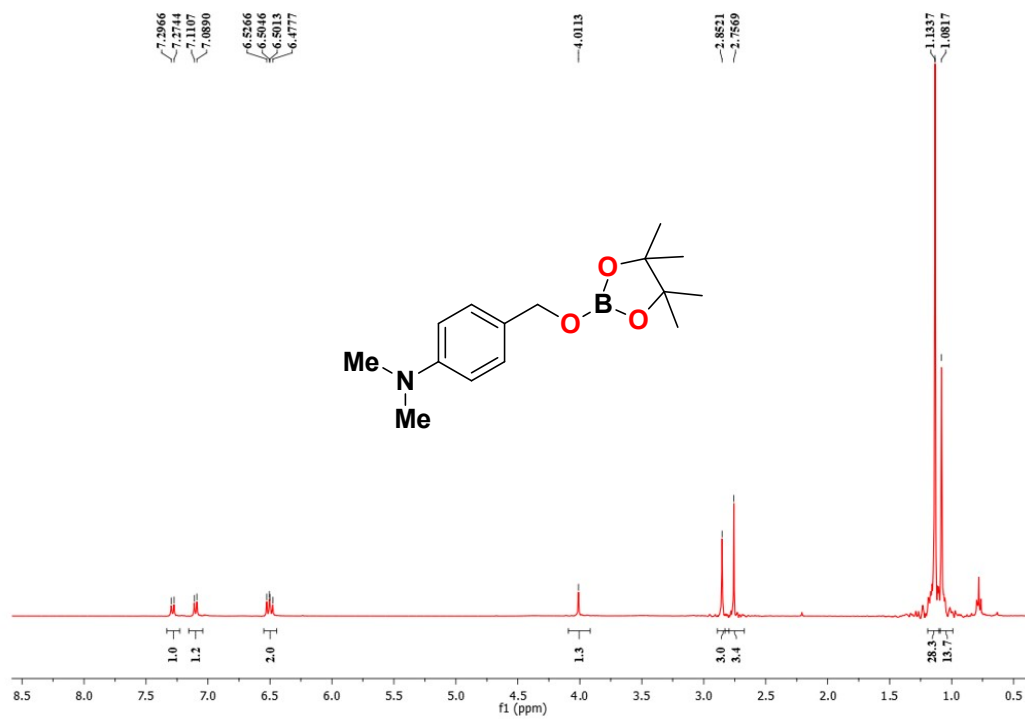
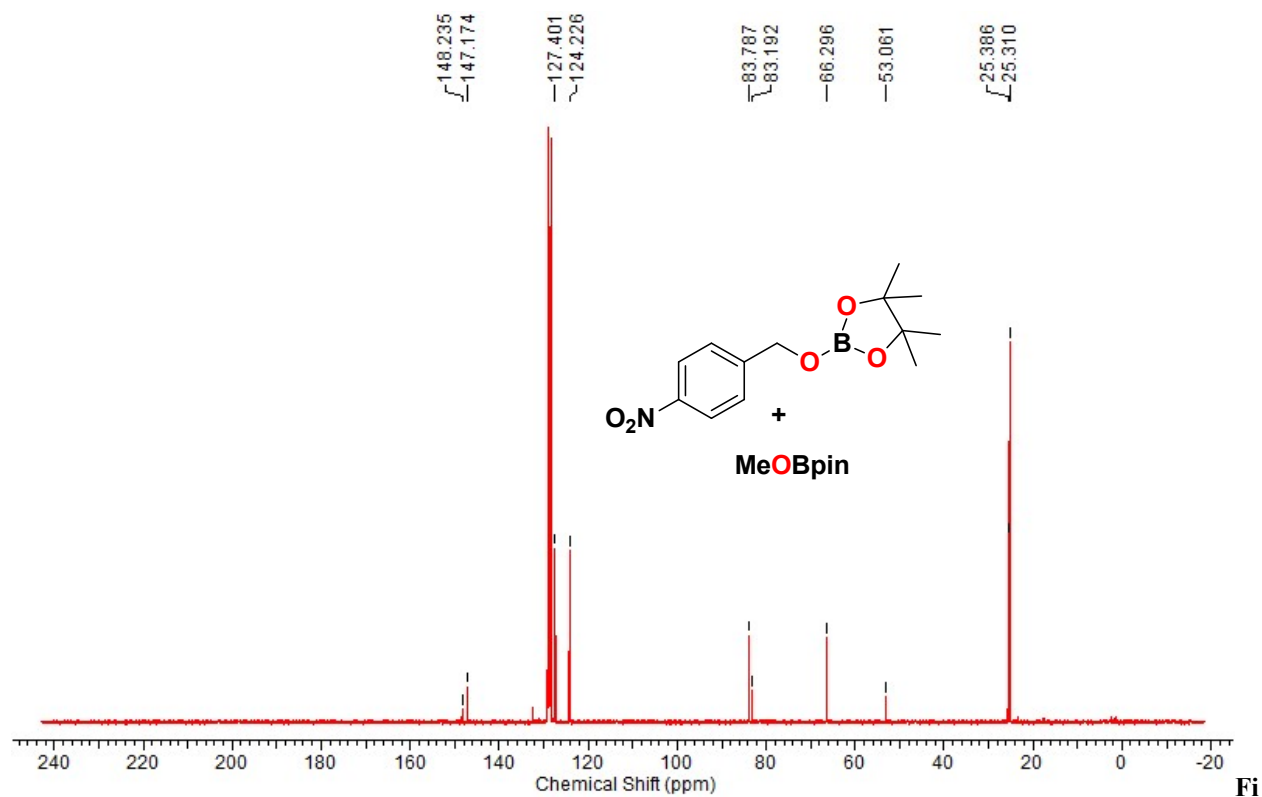


Figure S29. ^{11}B NMR spectrum (128.4 MHz, 25°C, C_6D_6) of compound **3h** and **3b**.



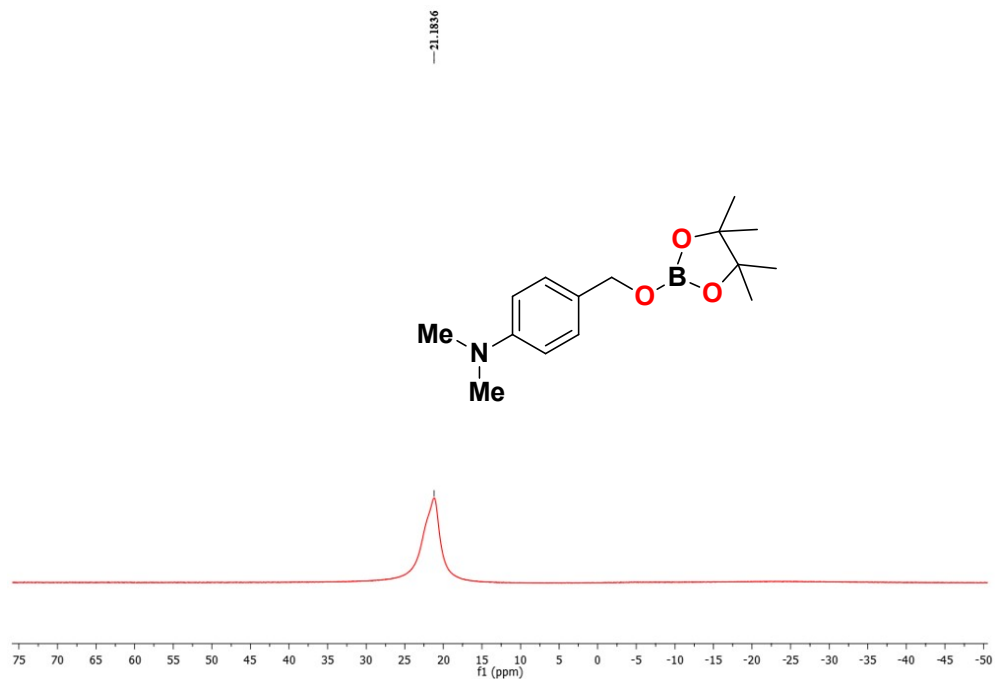


Figure S32. ^{11}B NMR spectrum (128.4 MHz, 25°C, CDCl_3) of compound **3i**.

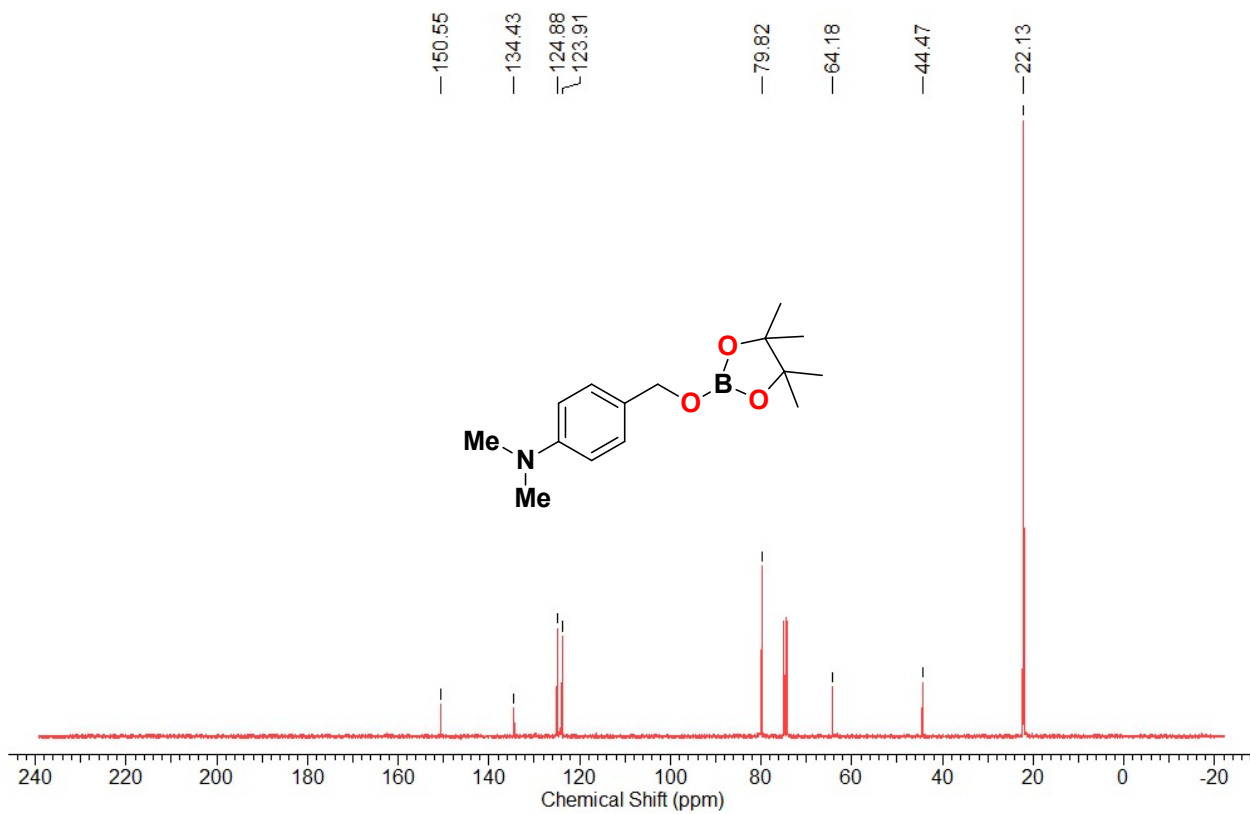


Figure S33. ^{13}C NMR spectrum (100 MHz, 25°C, CDCl_3) of compound **3i**.

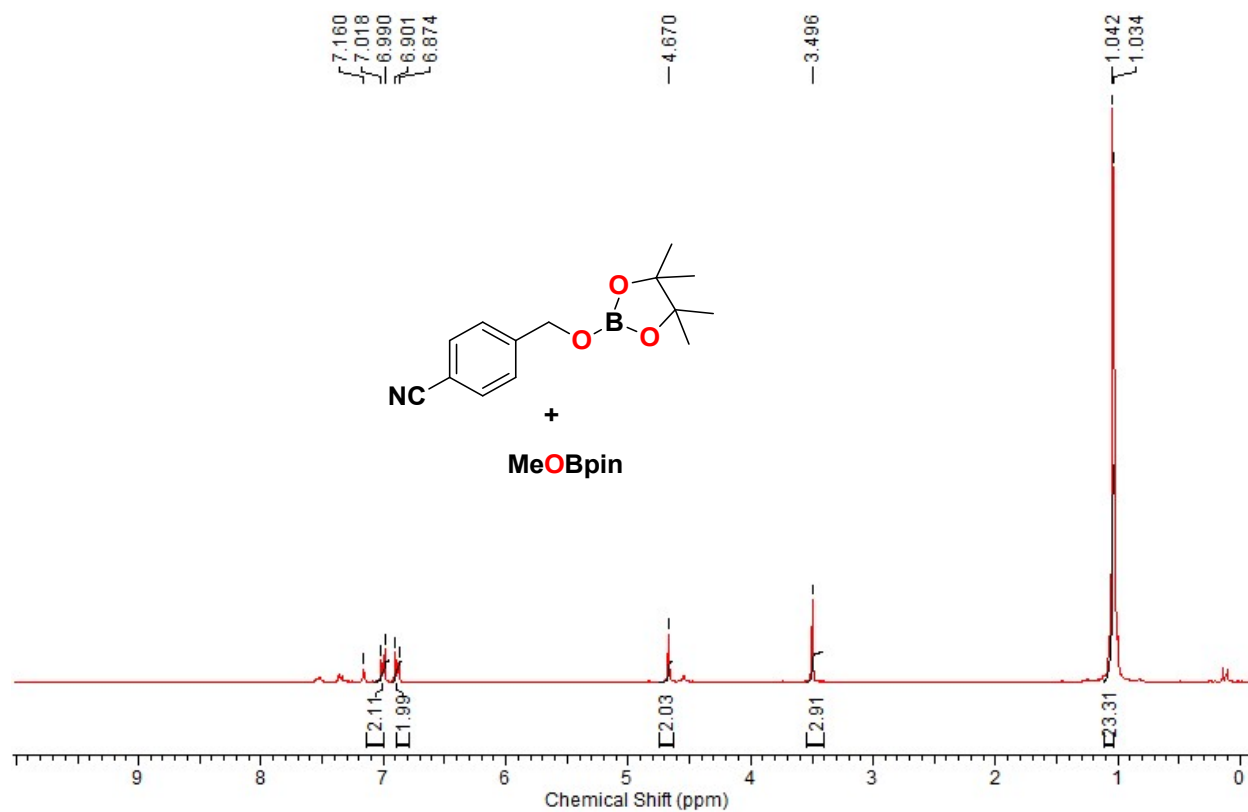


Figure S34. ^1H NMR spectrum (400 MHz, 25°C, CDCl_3) of compound **3j** and **3b**.

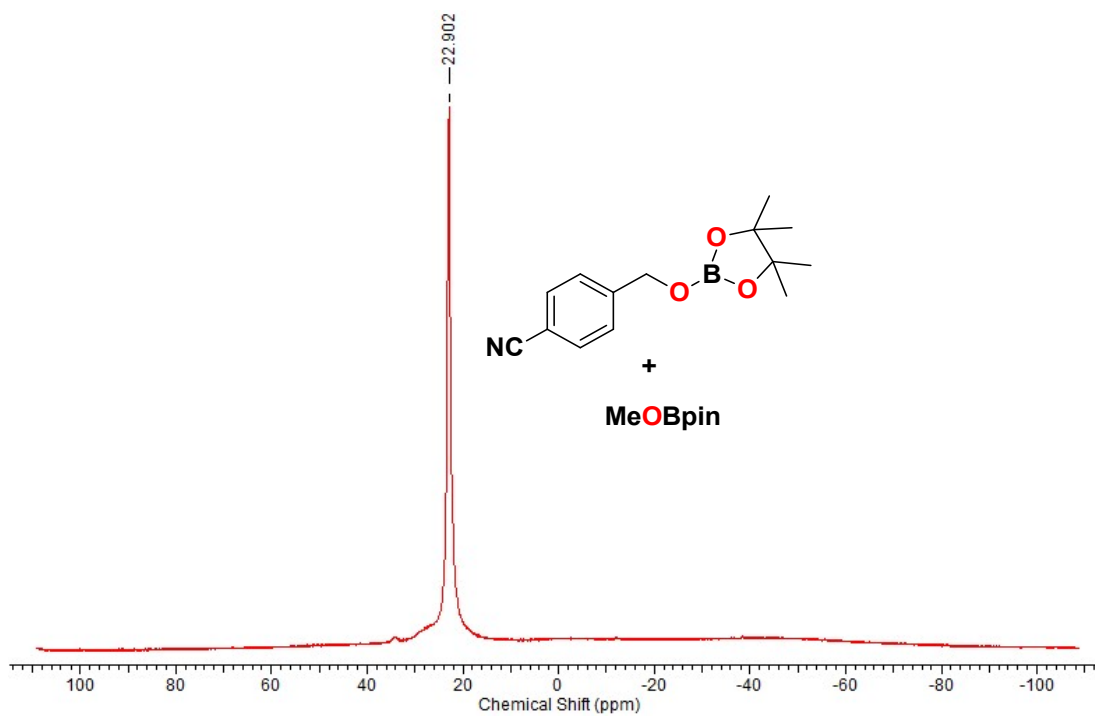


Figure S35. ^{11}B NMR spectrum (128.4 MHz, 25°C, CDCl_3) of **3j** and **3b**.

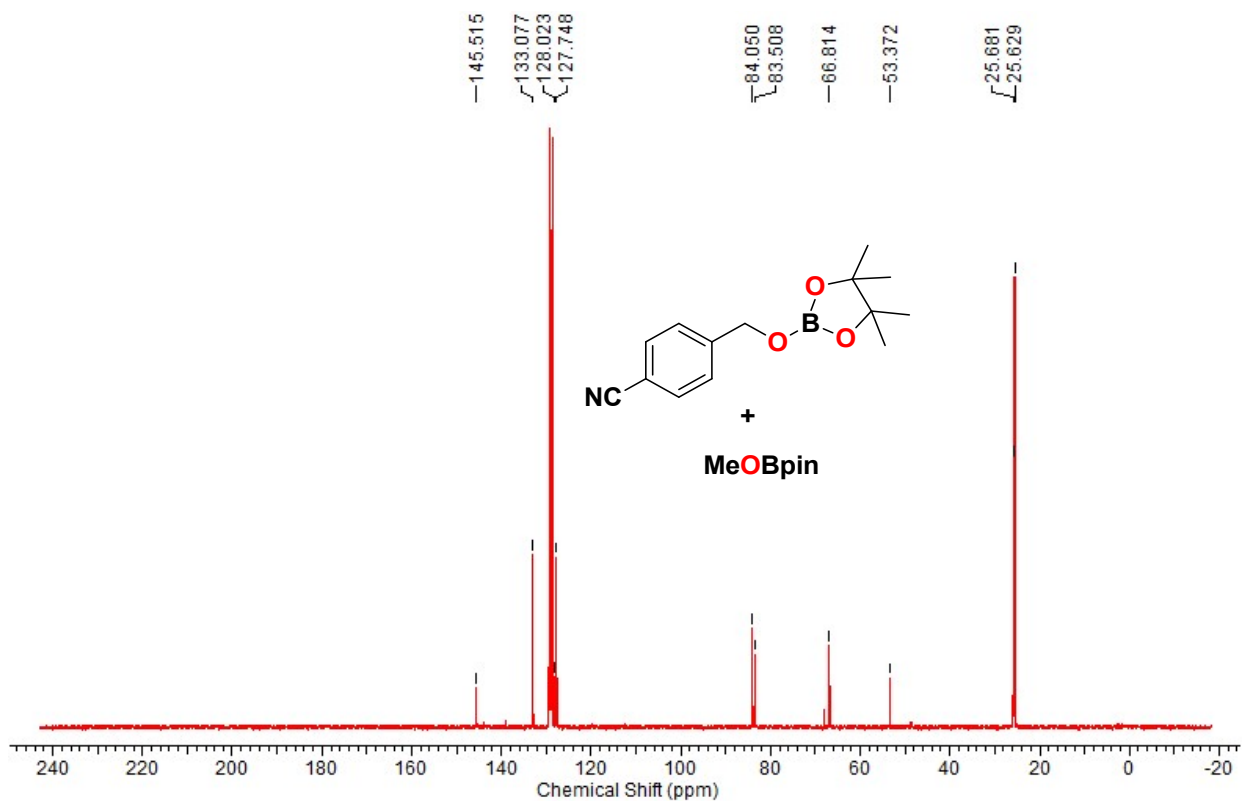


Figure S36. ^{13}C NMR spectrum (100 MHz, 25°C, CDCl_3) of compound **3j** and **3b**.

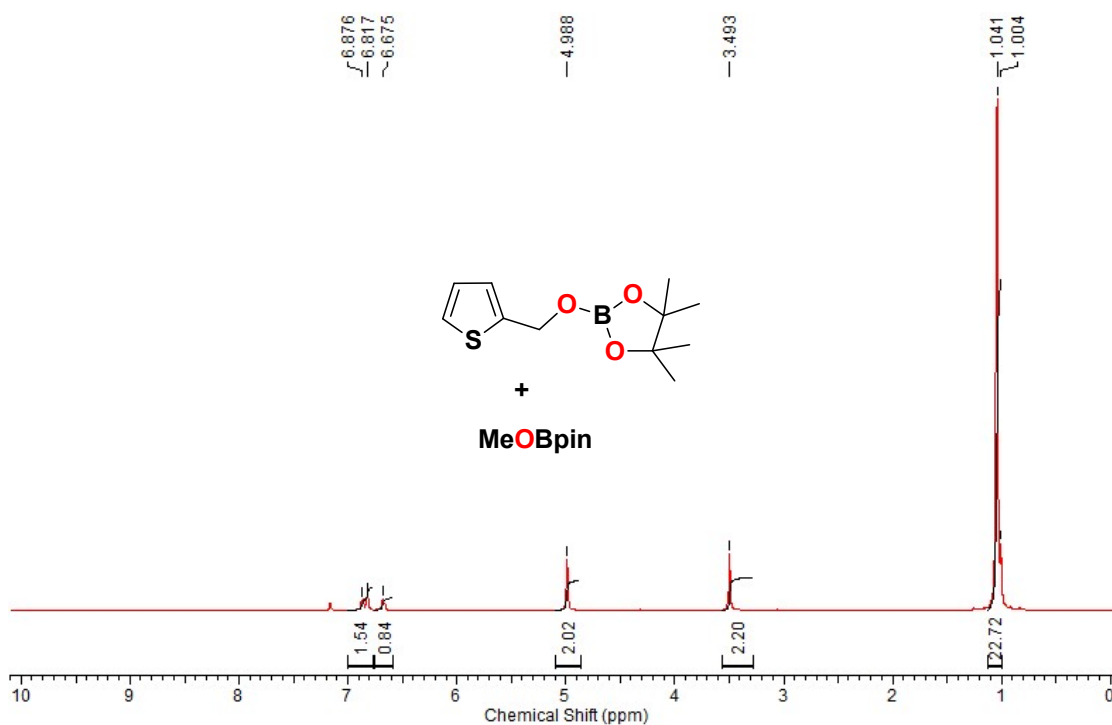


Figure S37. ^1H NMR spectrum (400 MHz, 25°C, C_6D_6) of compound **3k** and **3b**.

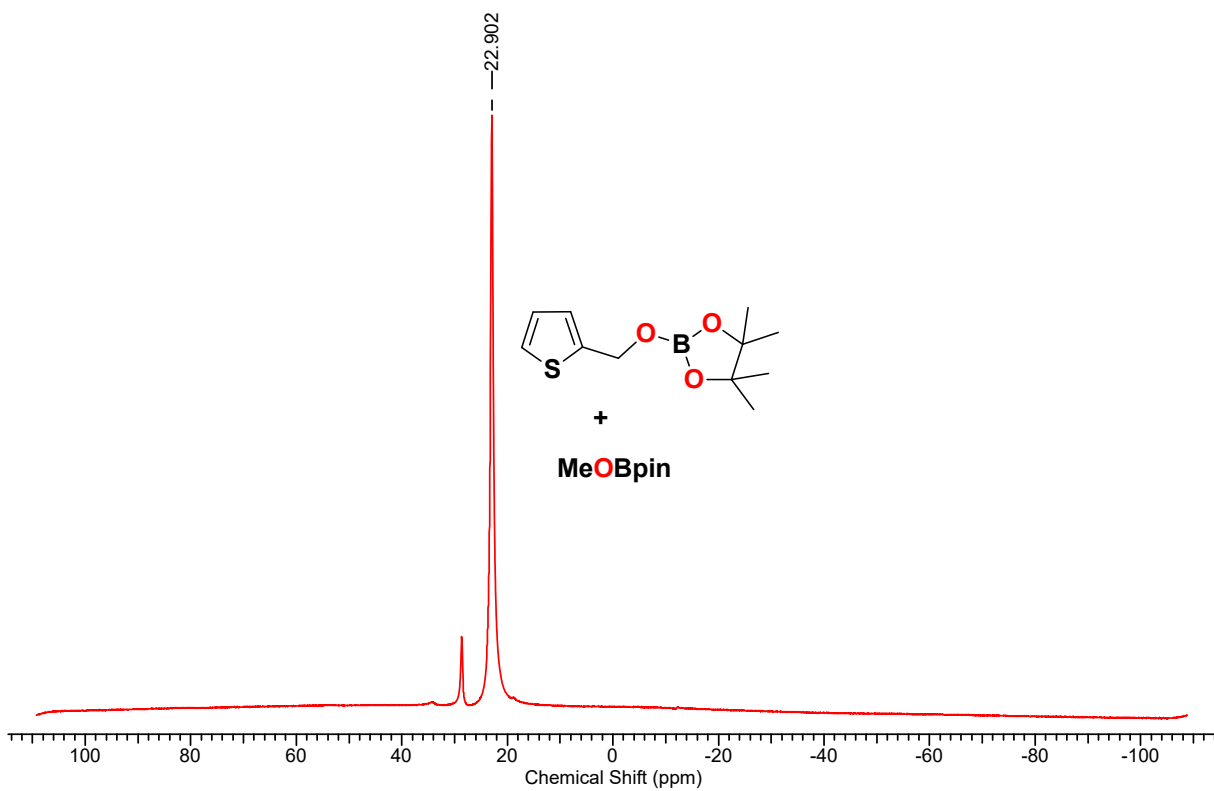


Figure S38. ^{11}B NMR spectrum (128.4 MHz, 25°C, C_6D_6) of compound **3k** and **3b**.

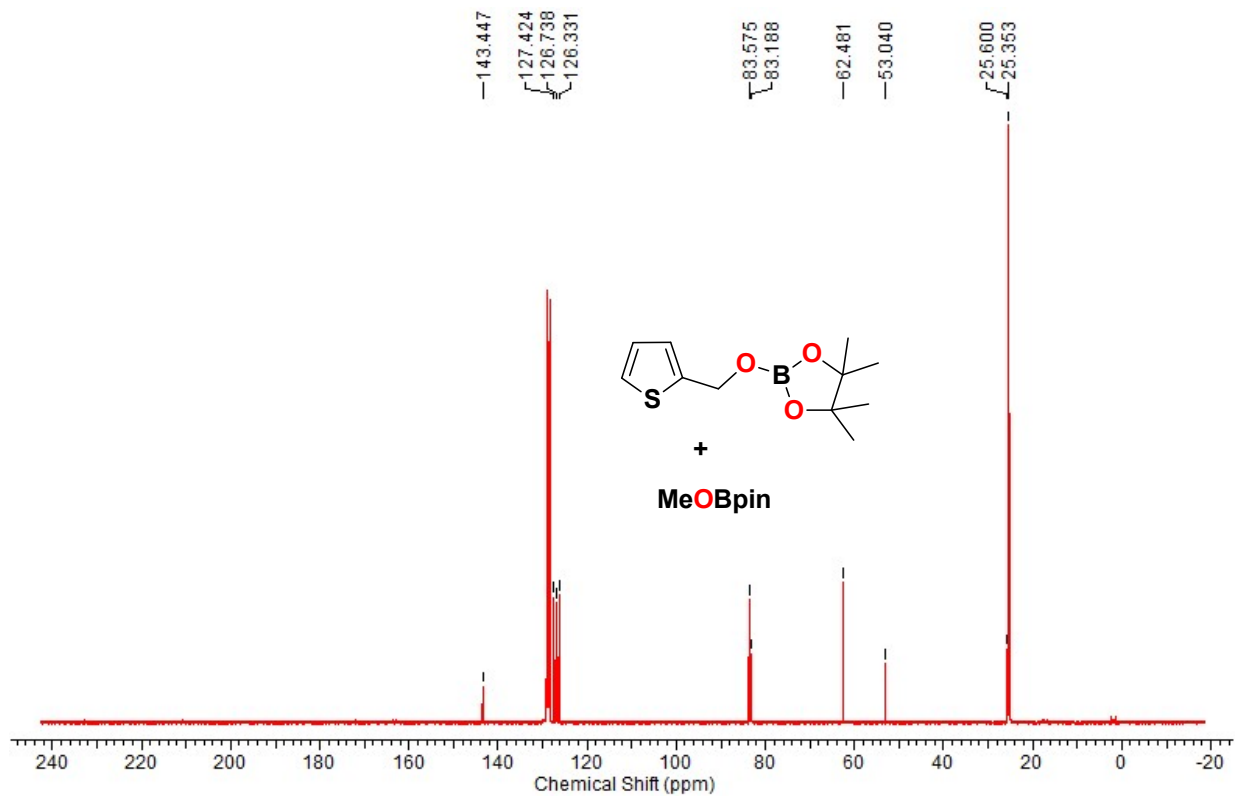


Figure S39. ^{13}C NMR spectrum (100 MHz, 25°C, C_6D_6) of compound **3k** and **3b**.

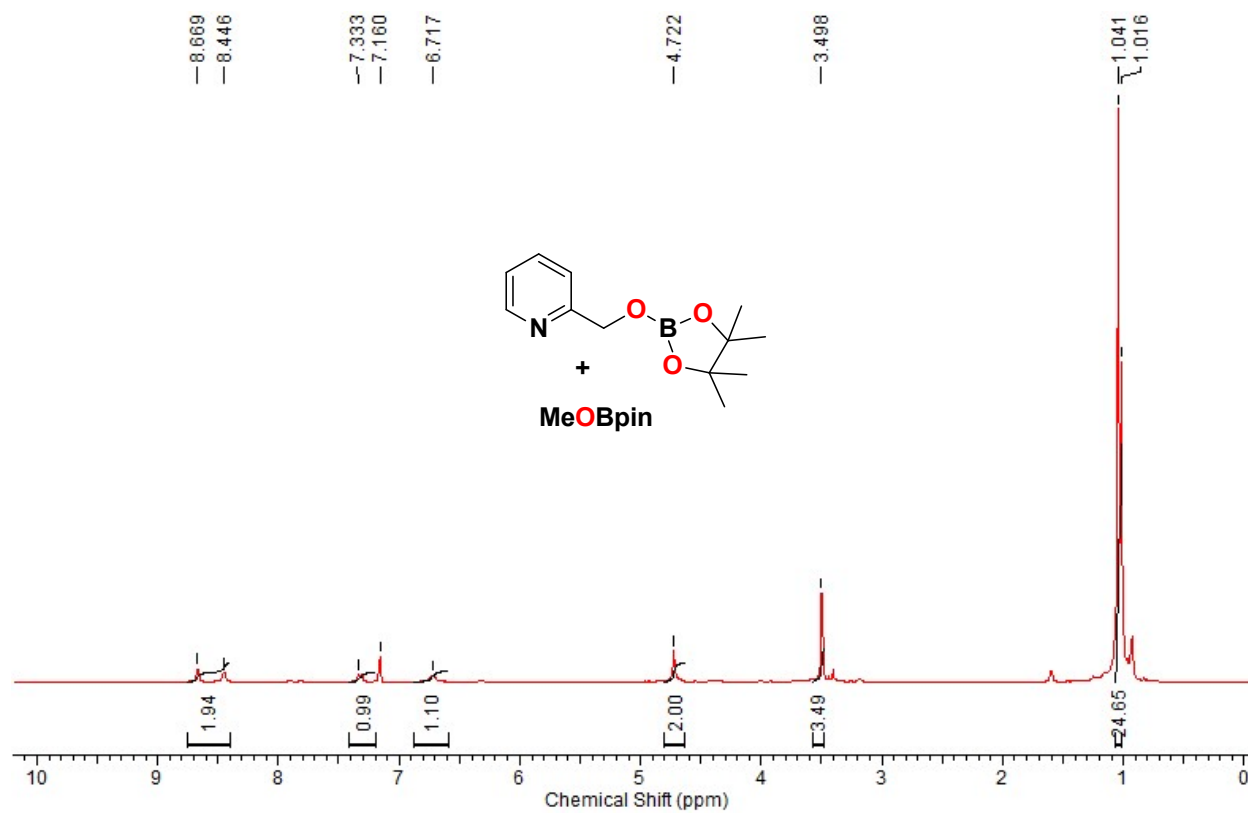


Figure S40. ¹H NMR spectrum (400 MHz, 25°C, CDCl₃) of compound **31** and **3b**.

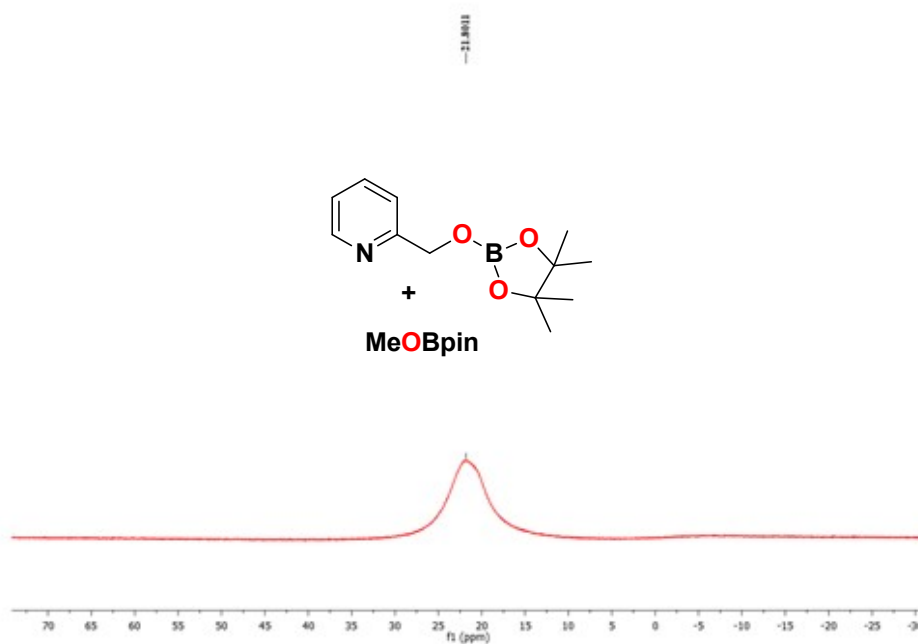


Figure S41. ¹¹B NMR spectrum (128.4 MHz, 25°C, CDCl₃) of compound **31** and **3b**.

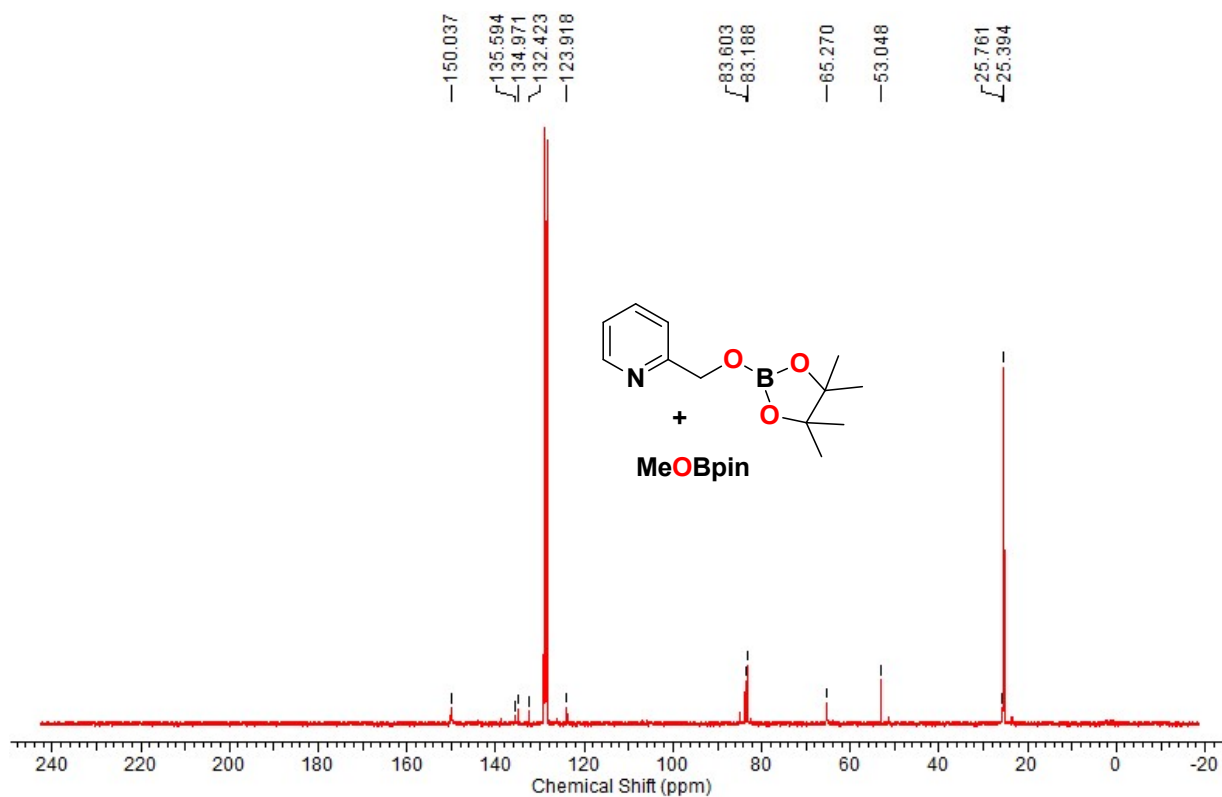


Figure S42. ^{13}C NMR spectrum (400 MHz, 25°C, CDCl_3) of compound **3l** and **3b**.

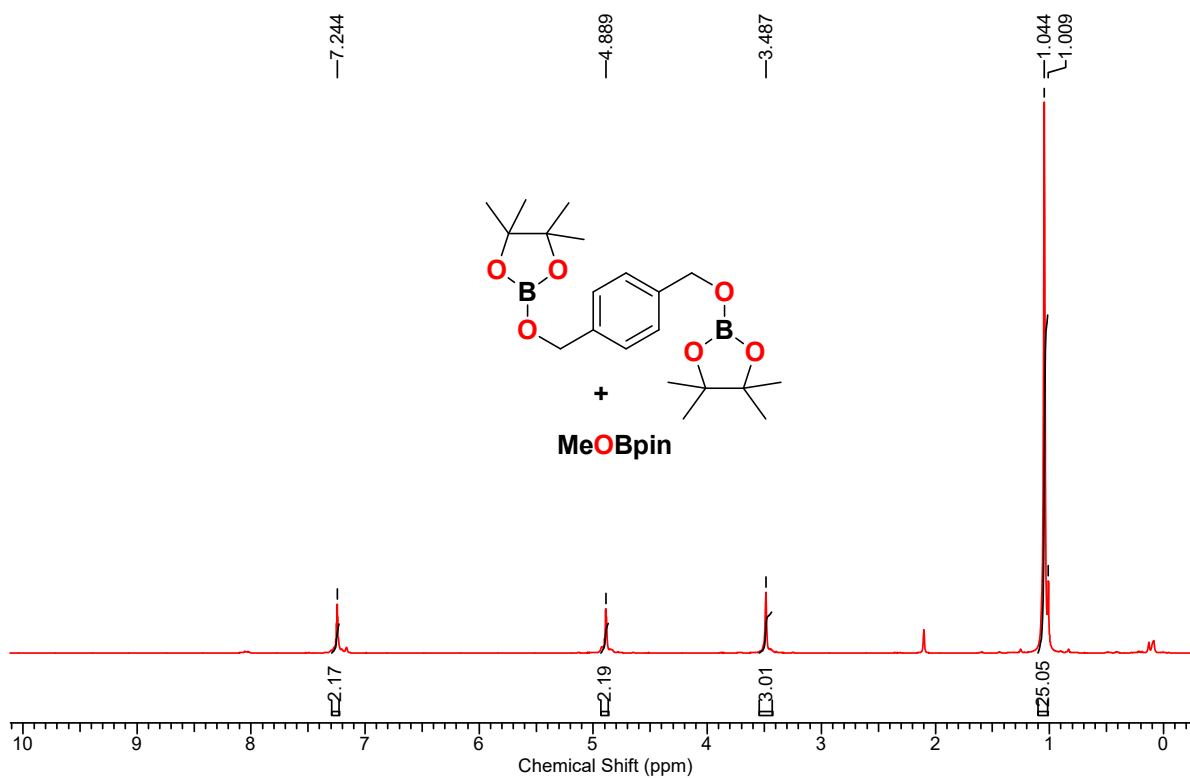


Figure S43. ^1H NMR spectrum (400 MHz, 25°C, CDCl_3) of compound **3m** and **3b**.

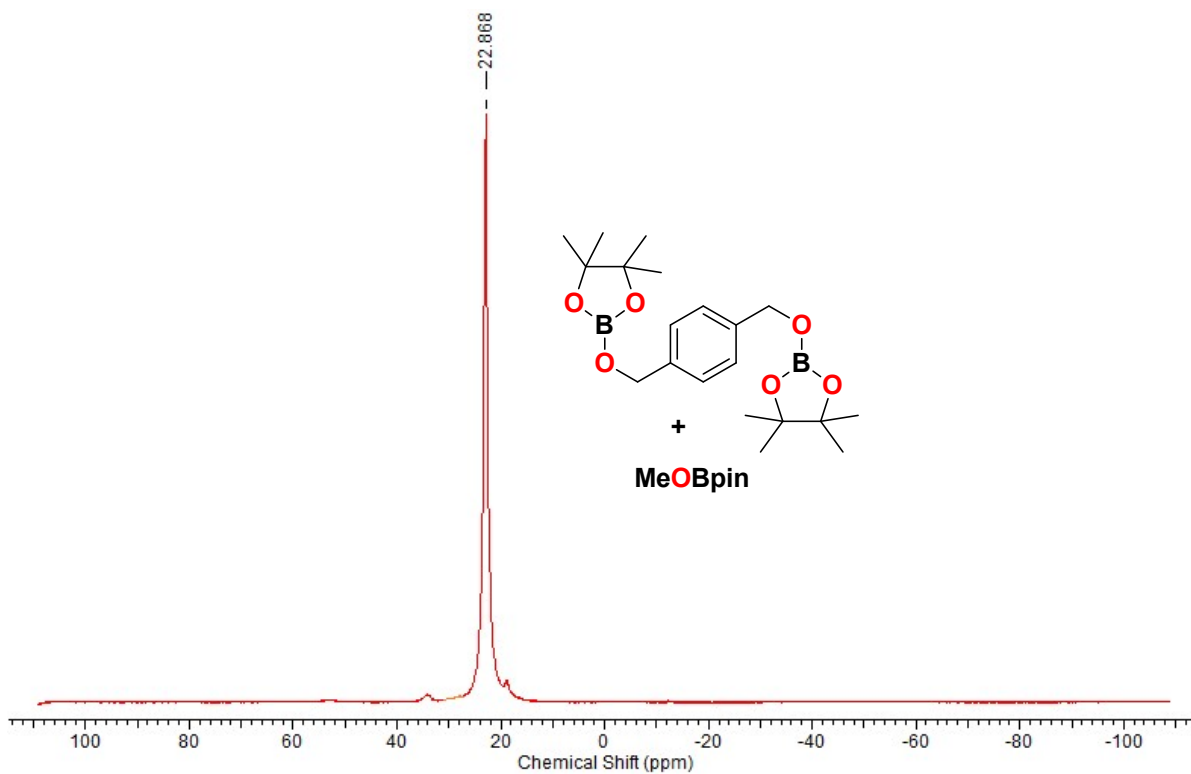


Figure S44. ^{11}B NMR spectrum (128.4 MHz, 25°C, CDCl_3) of compound **3m** and **3b**.

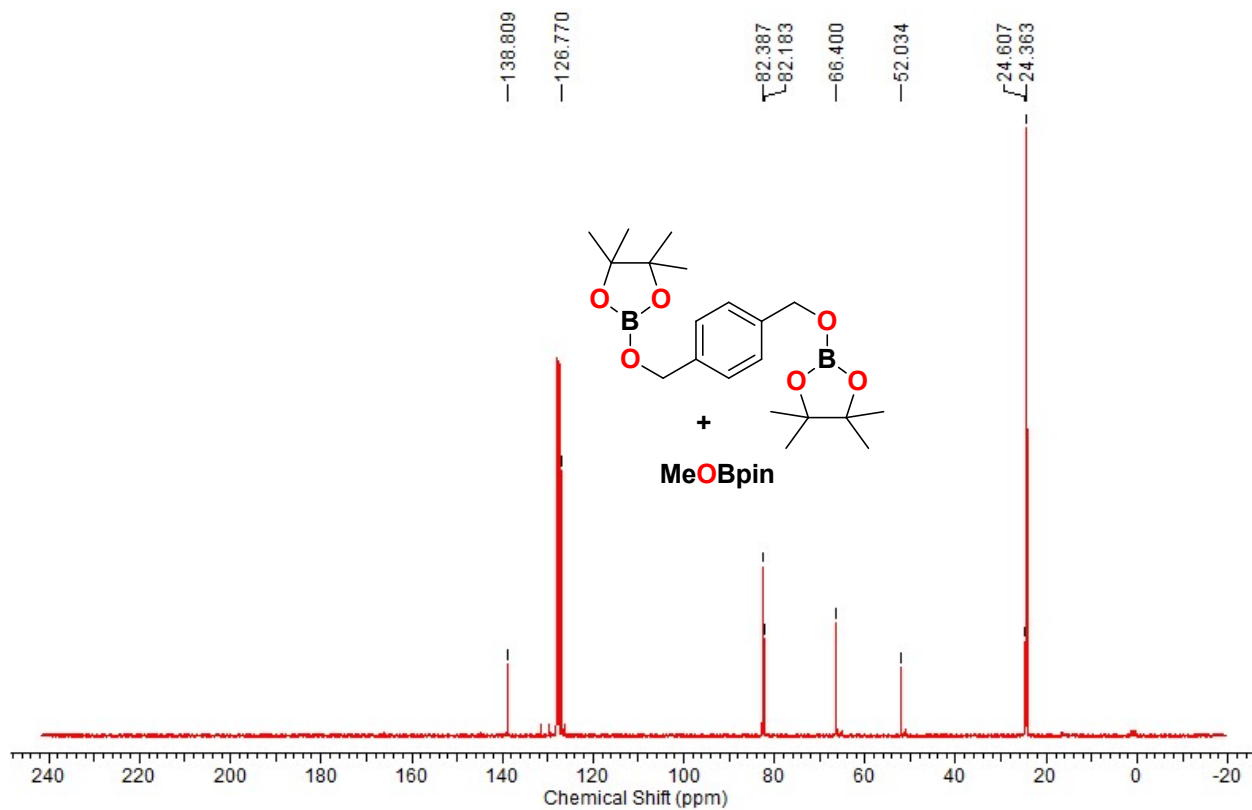


Figure S45. ^{13}C NMR spectrum (100 MHz, 25°C, CDCl_3) of compound **3m** and **3b**.

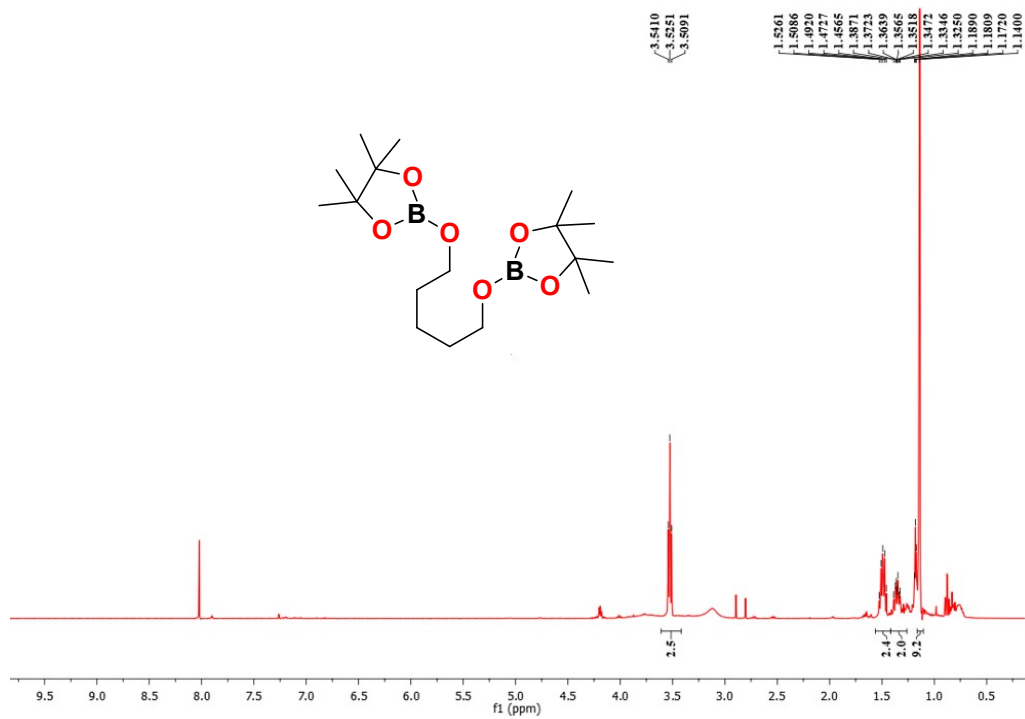


Figure S46. ^1H NMR spectrum (400 MHz, 25°C, CDCl_3) of compound **3n**.

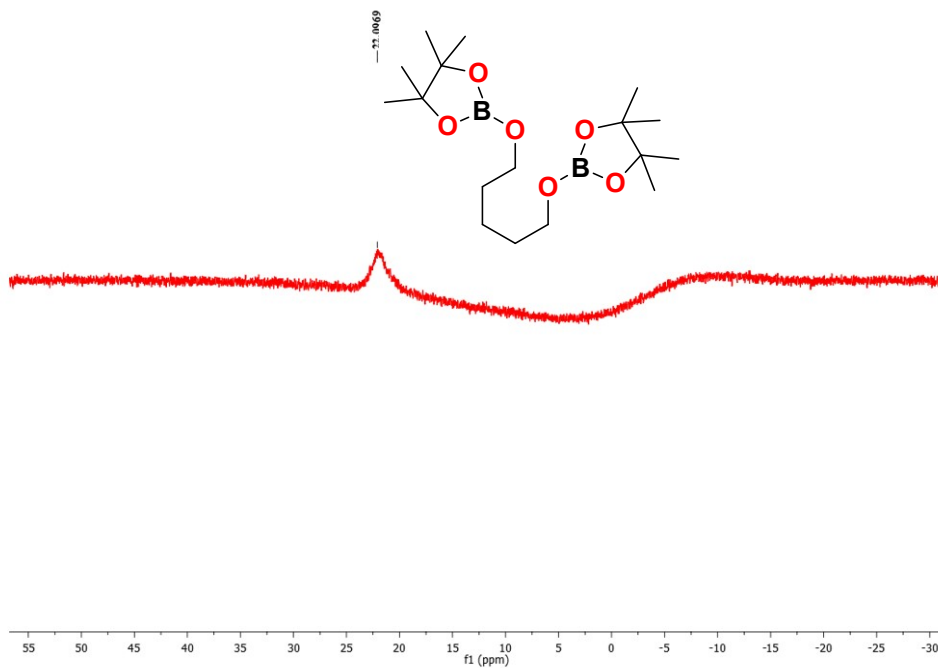


Figure S47. ^{11}B NMR spectrum (128.4 MHz, 25°C, CDCl_3) of compound **3n**.

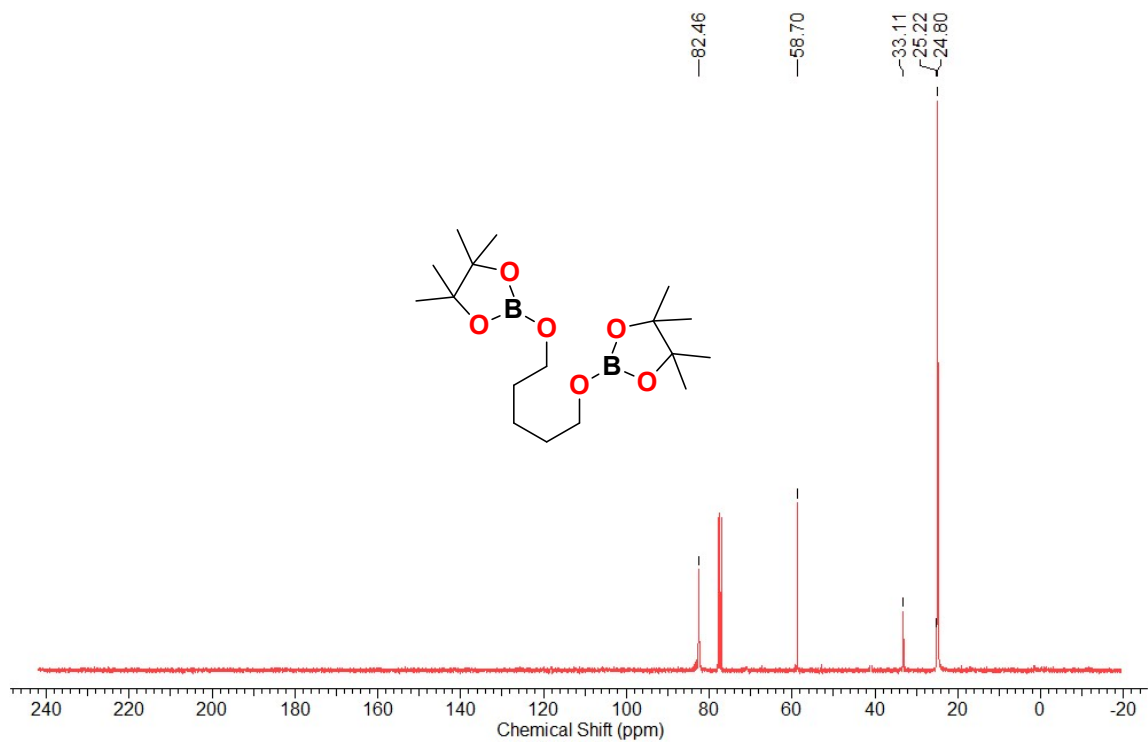


Figure S48. ^{13}C NMR spectrum (100 MHz, 25°C , CDCl_3) of compound **3n**.

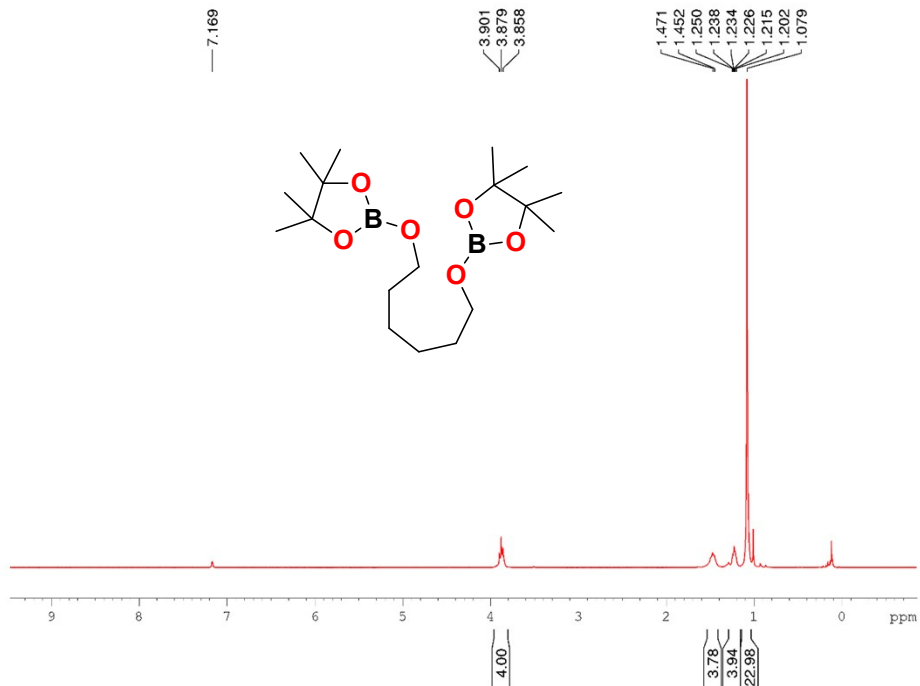


Figure S49. ^1H NMR spectrum (400 MHz, 25°C , C_6D_6) of compound **3o**.

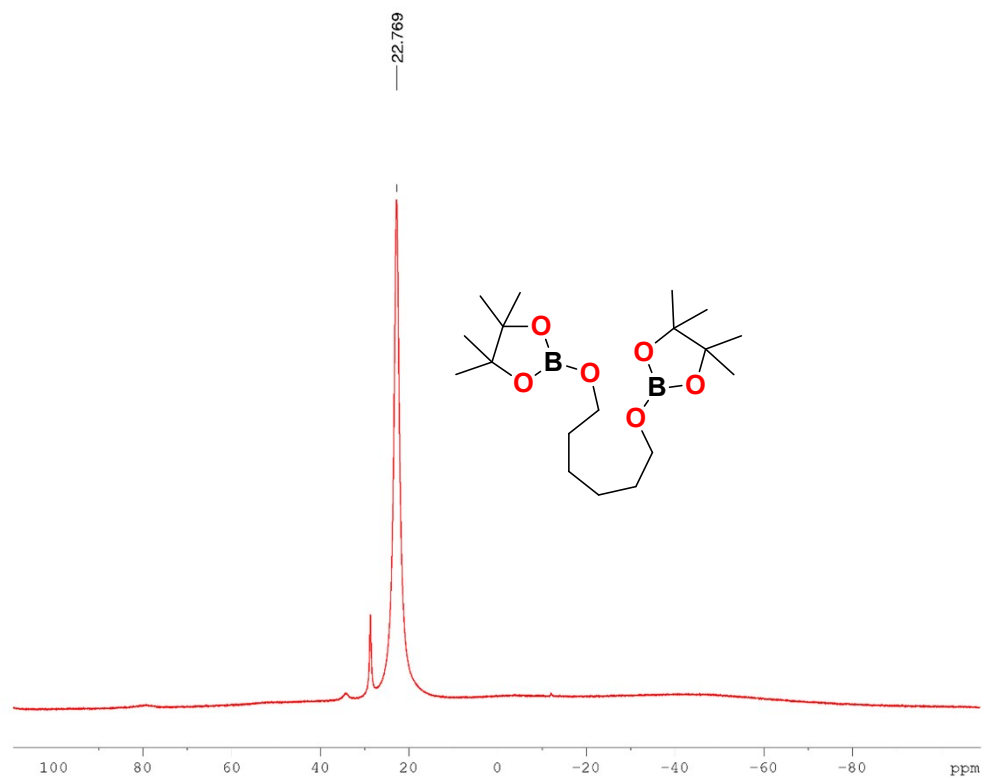


Figure S50. ¹¹B NMR spectrum (128.4 MHz, 25°C, C₆D₆) of compound **3o**.

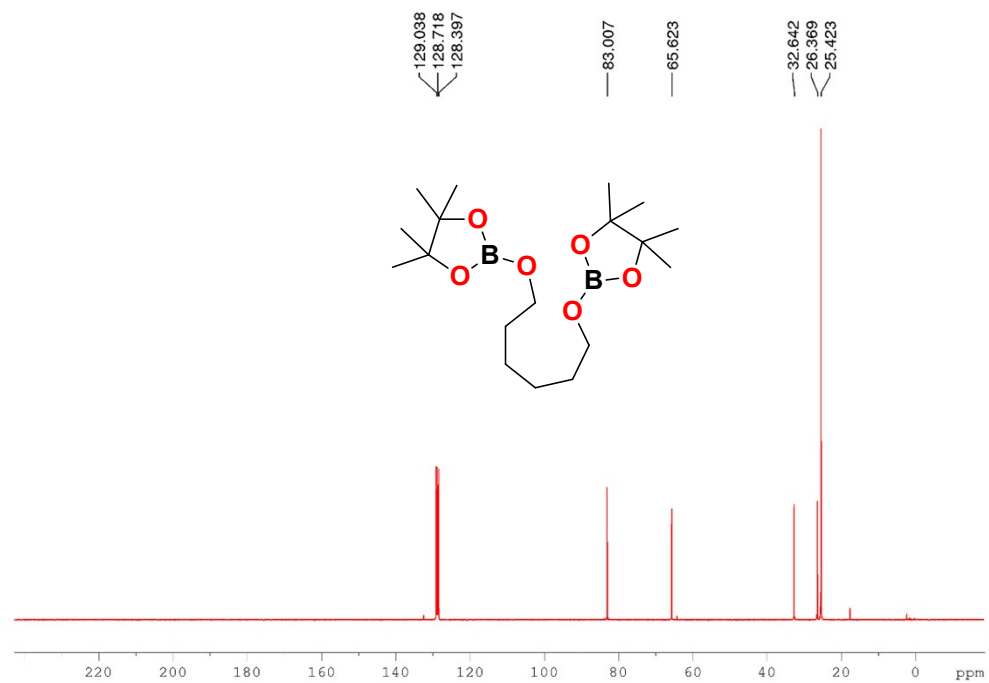


Figure S51. ¹³C NMR spectrum (100 MHz, 25°C, C₆D₆) of compound **3o**.

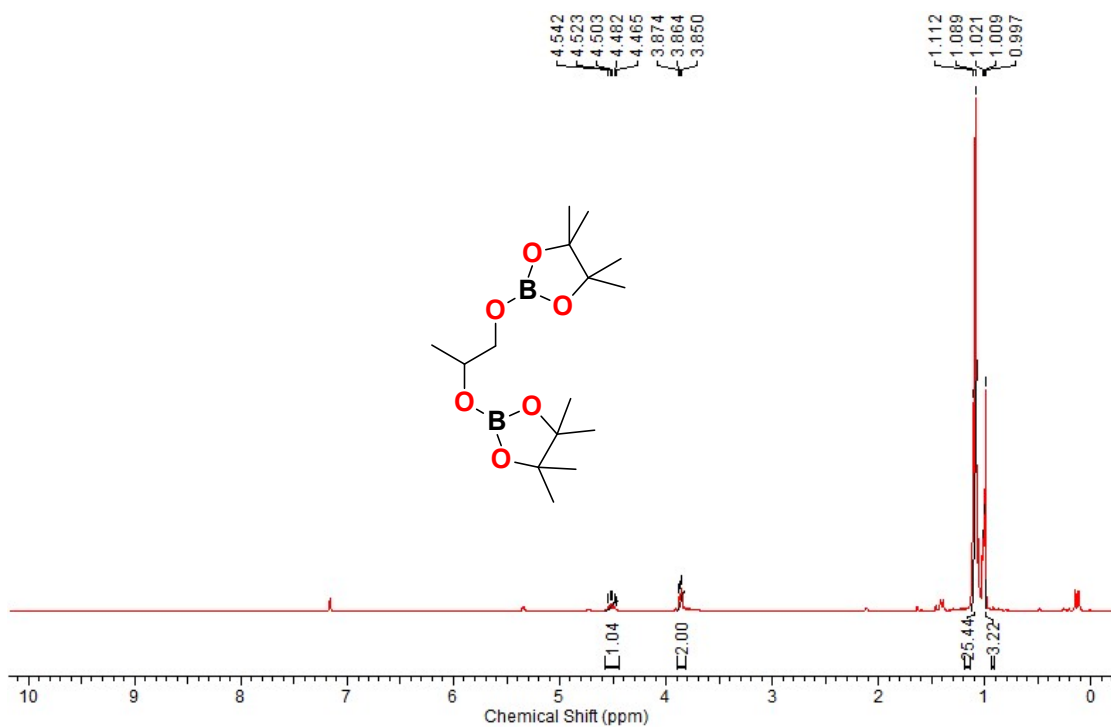


Figure S52. ^1H NMR spectrum (400 MHz, 25°C , C_6D_6) of compound $2 \times 3\text{p}$.

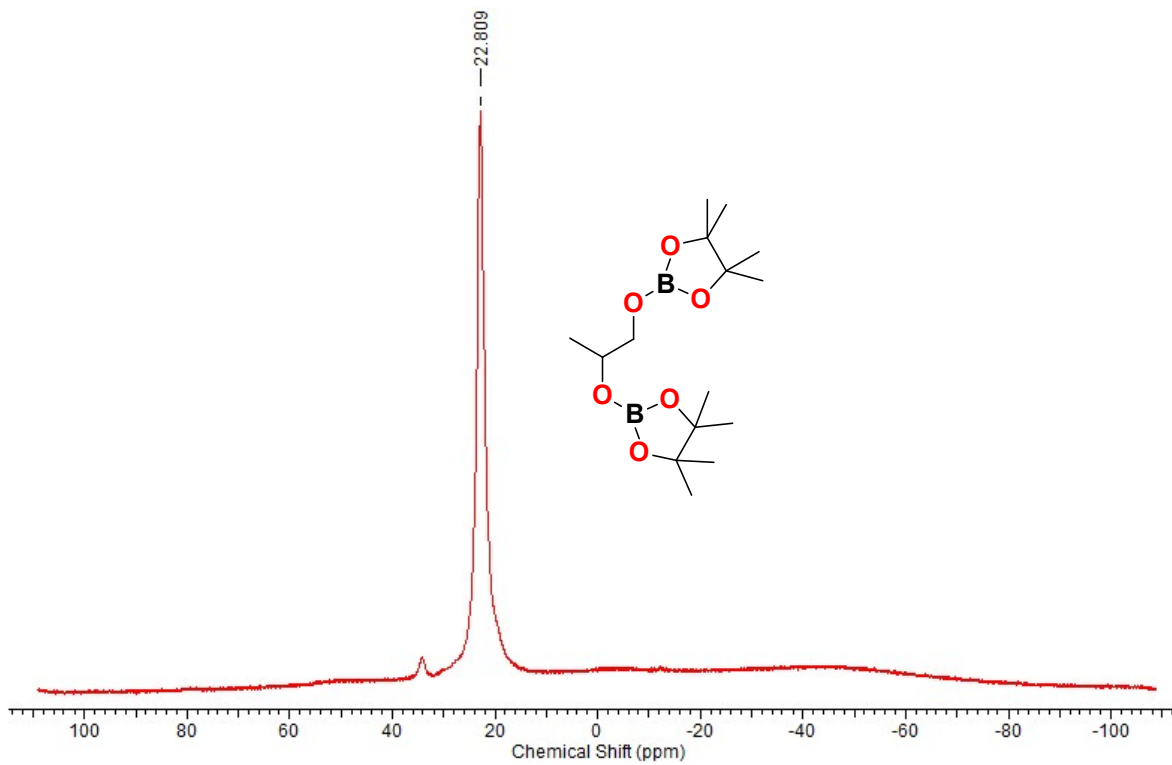


Figure S53. ^{11}B NMR spectrum (128.4 MHz, 25°C , C_6D_6) of compound $2 \times 3\text{p}$.

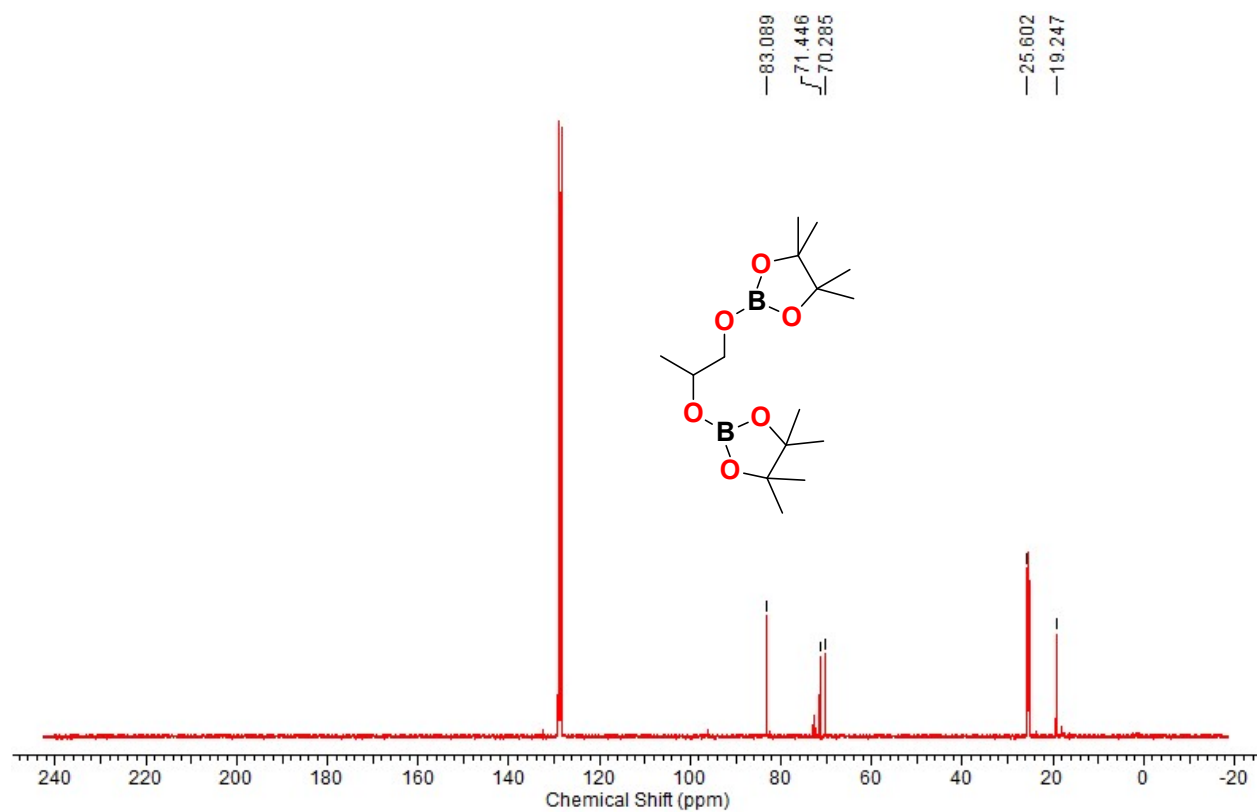


Figure S54. ^{13}C NMR spectrum (100 MHz, 25°C, C_6D_6) of compound 2 x 3p.

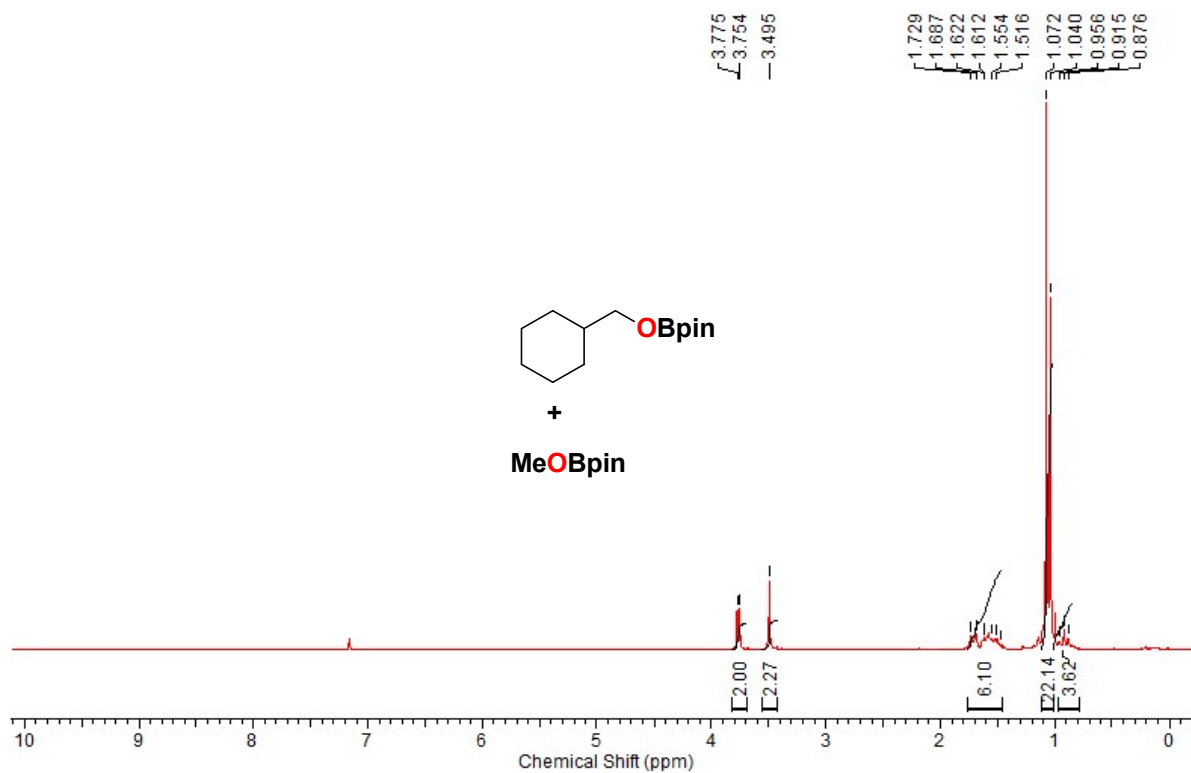


Figure S55. ^1H NMR spectrum (400 MHz, 25°C, C_6D_6) of compound 3q and 3b.

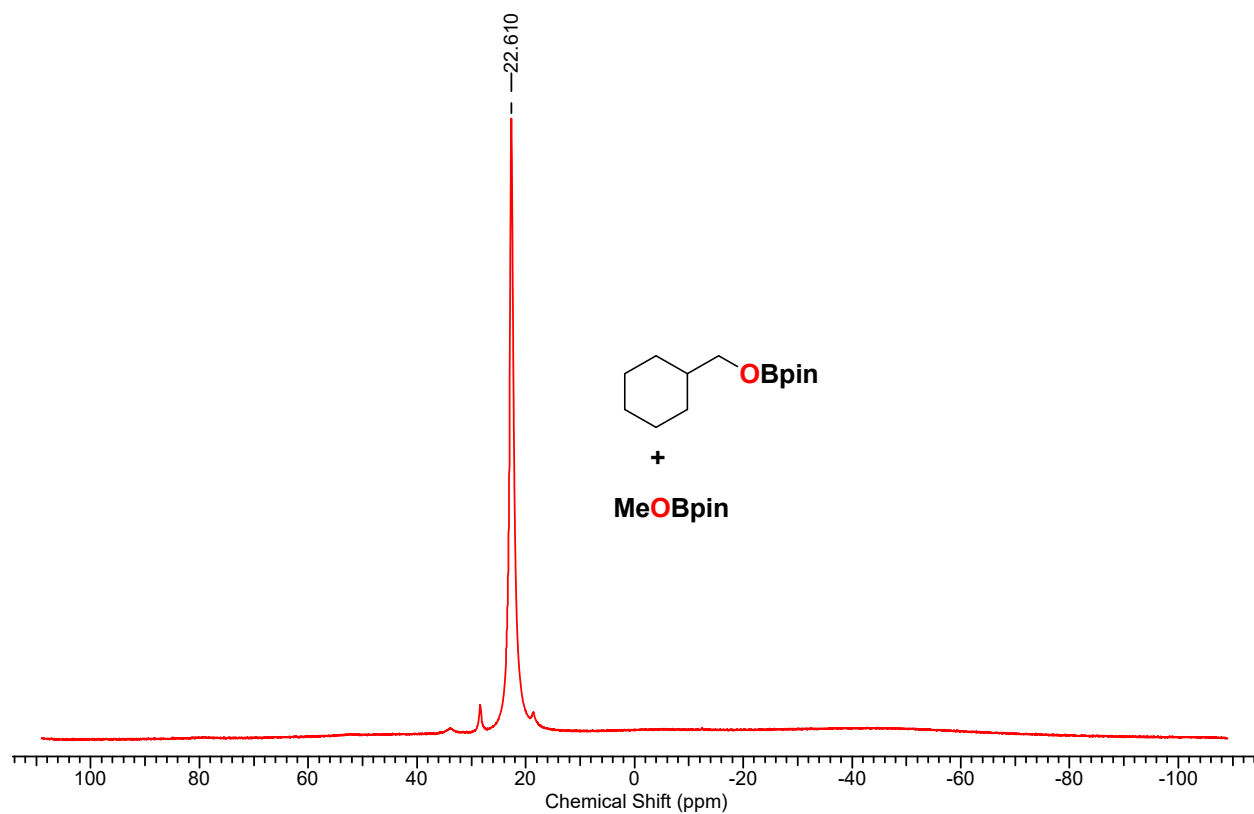


Figure S56. ^{11}B NMR spectrum (128.4 MHz, 25°C, C_6D_6) of compound **3q** and **3b**.

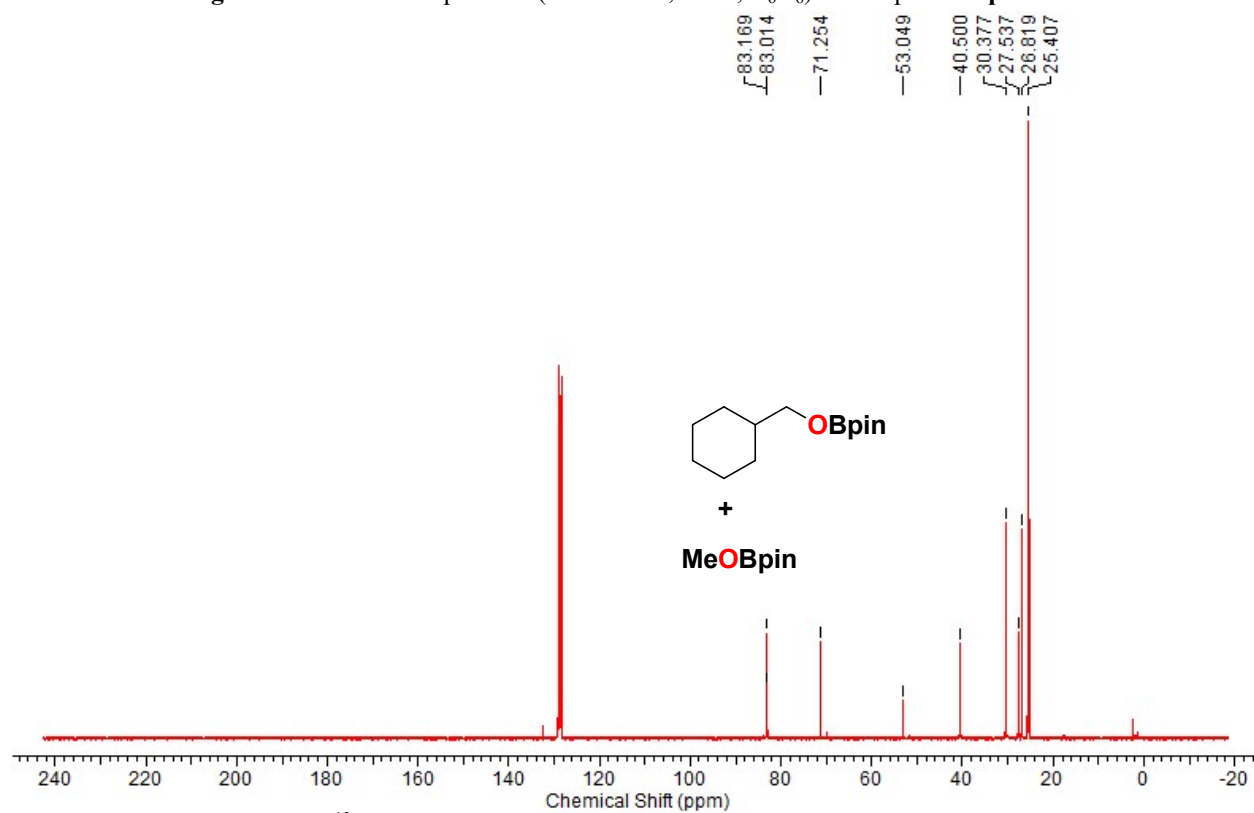


Figure S57. ^{13}C NMR spectrum (100 MHz, 25°C, C_6D_6) of compound **3q** and **3b**.

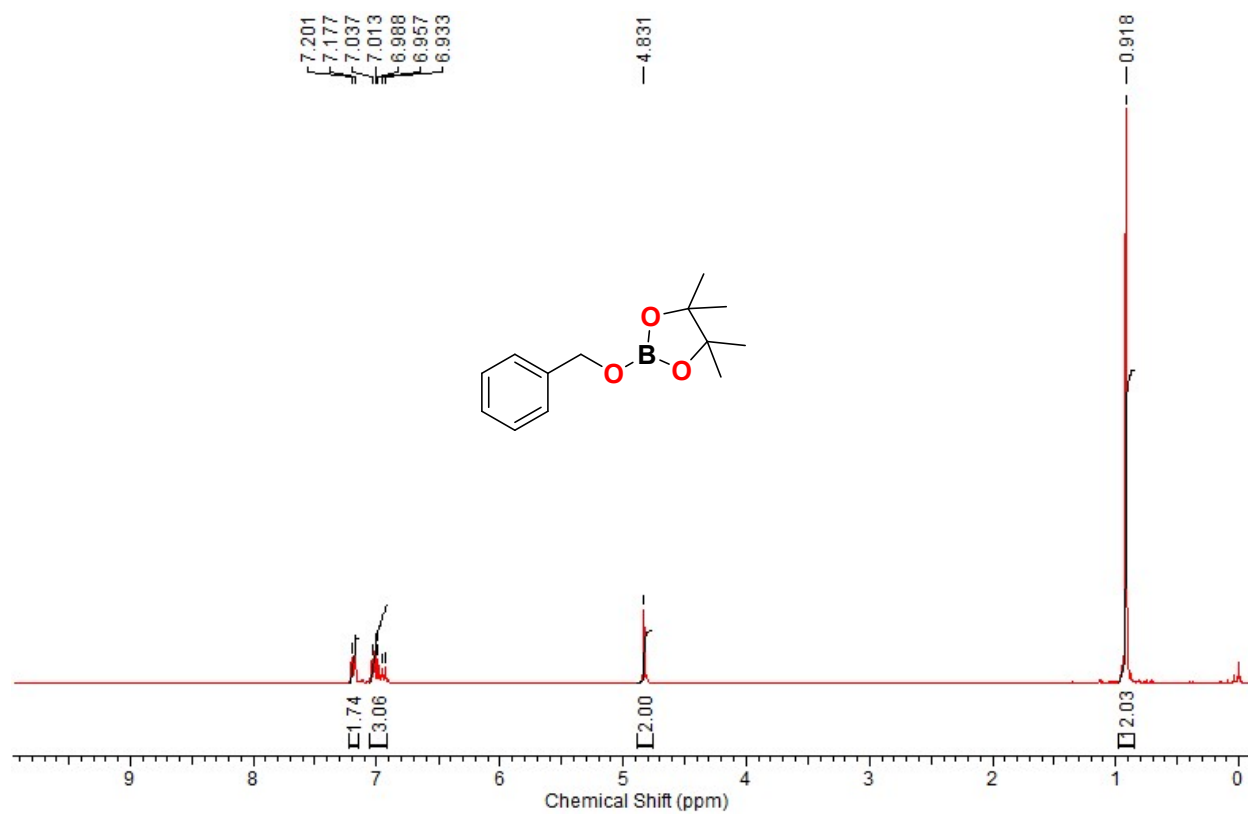


Figure S58. ¹H NMR spectrum (100 MHz, 25°C, C₆D₆) of compound 2 x 3a.

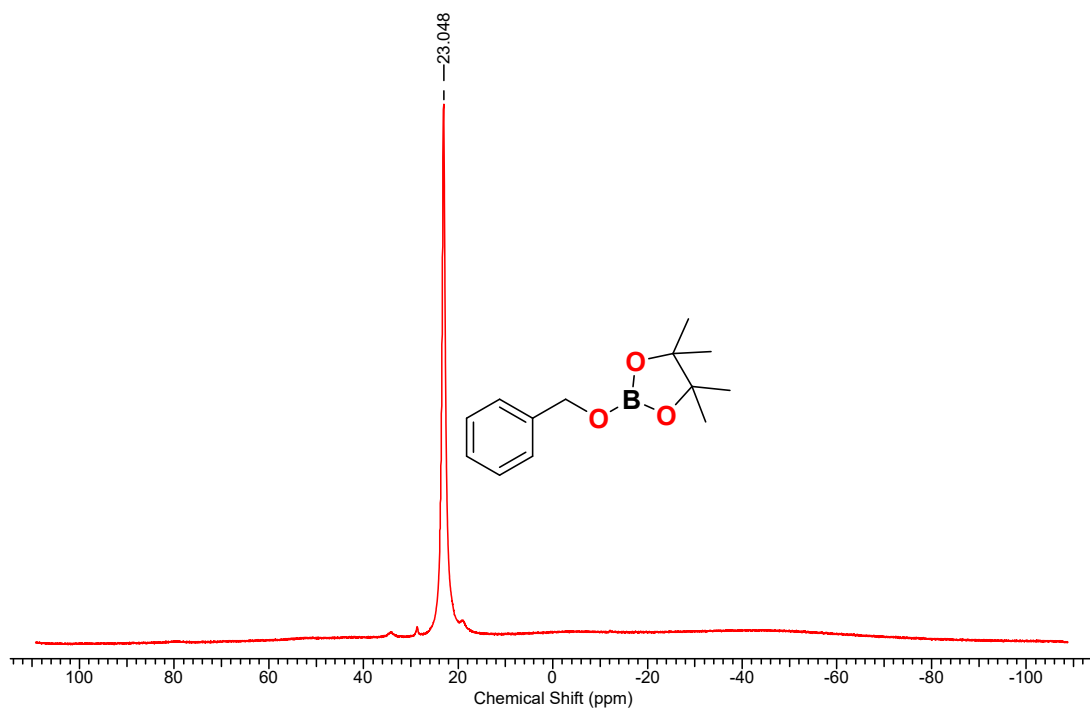


Figure S59. ¹¹B NMR spectrum (128.4 MHz, 25°C, C₆D₆) of compound 2 x 3a.

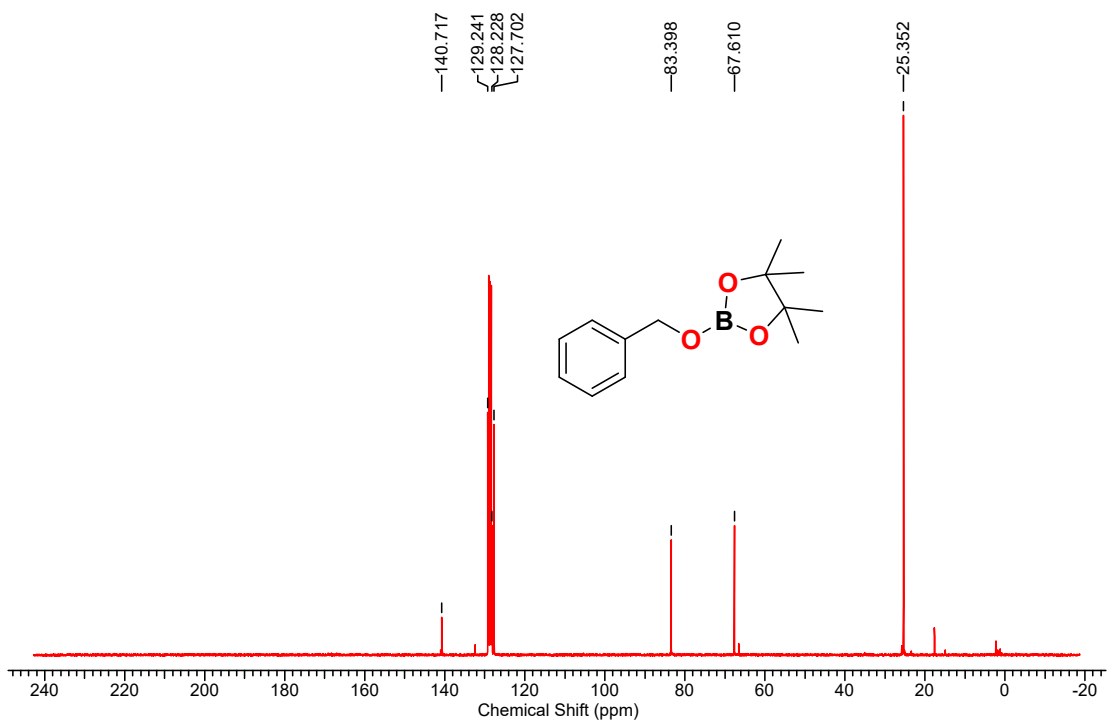


Figure S60. ^{13}C NMR spectrum (100 MHz, 25°C , C_6D_6) of compound 2 x **3a**.

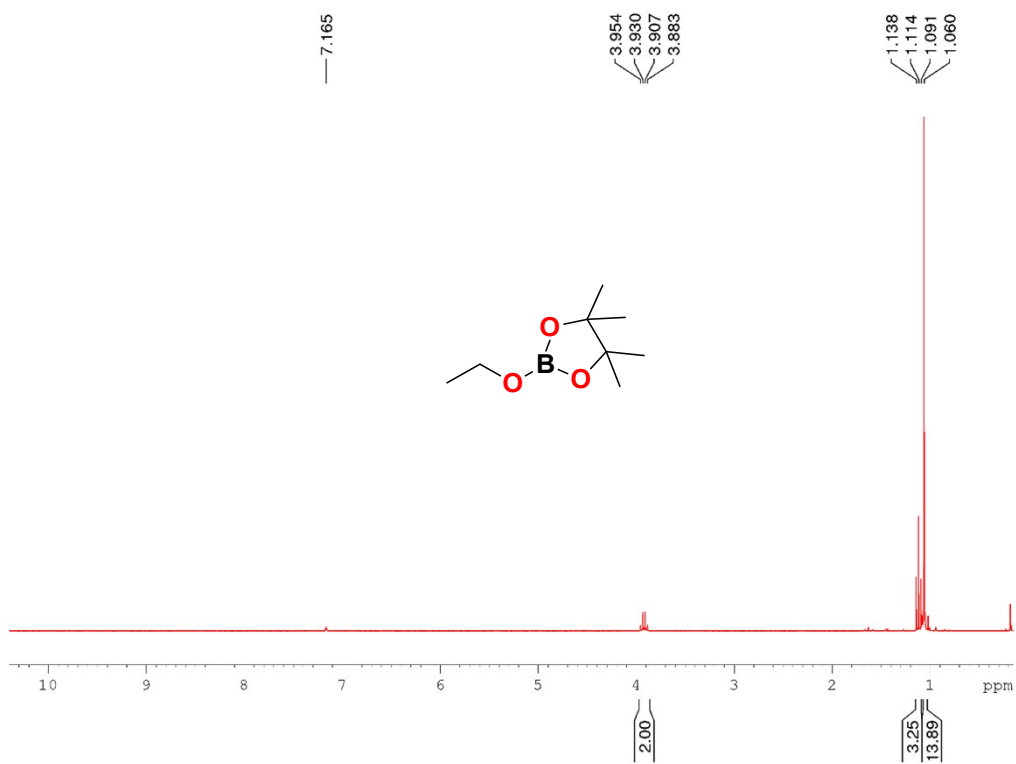


Figure S61. ^1H NMR spectrum (400 MHz, 25°C , C_6D_6) of compound 2 x **3r**.

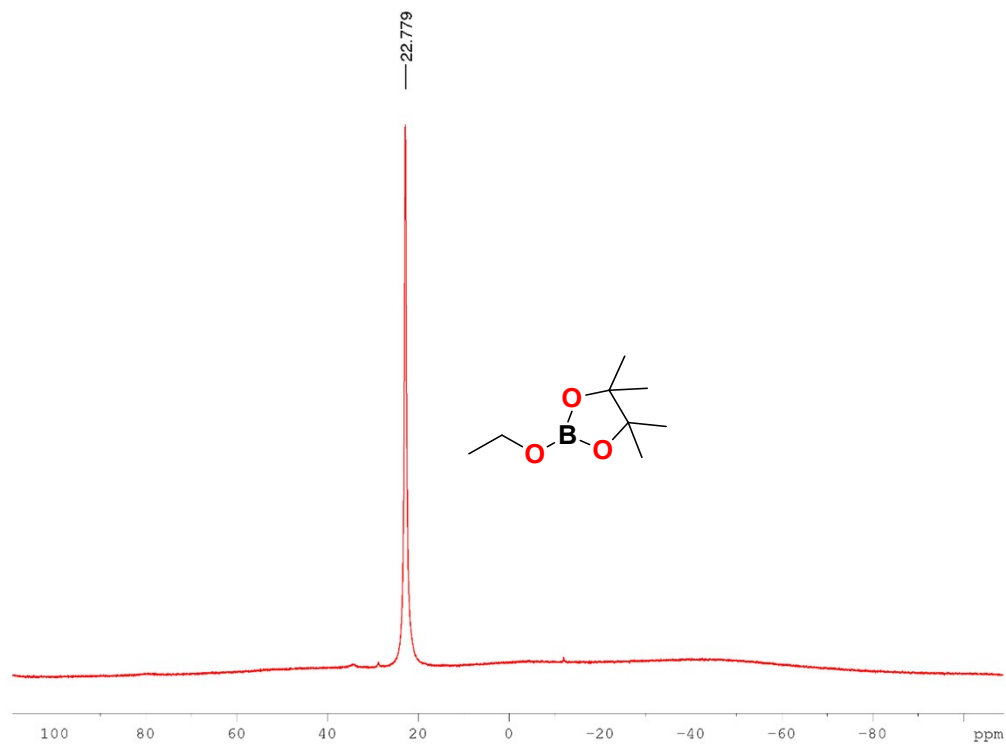


Figure S62. ^{11}B NMR spectrum (128.4 MHz, 25°C, C_6D_6) of compound **2 x 3r**.

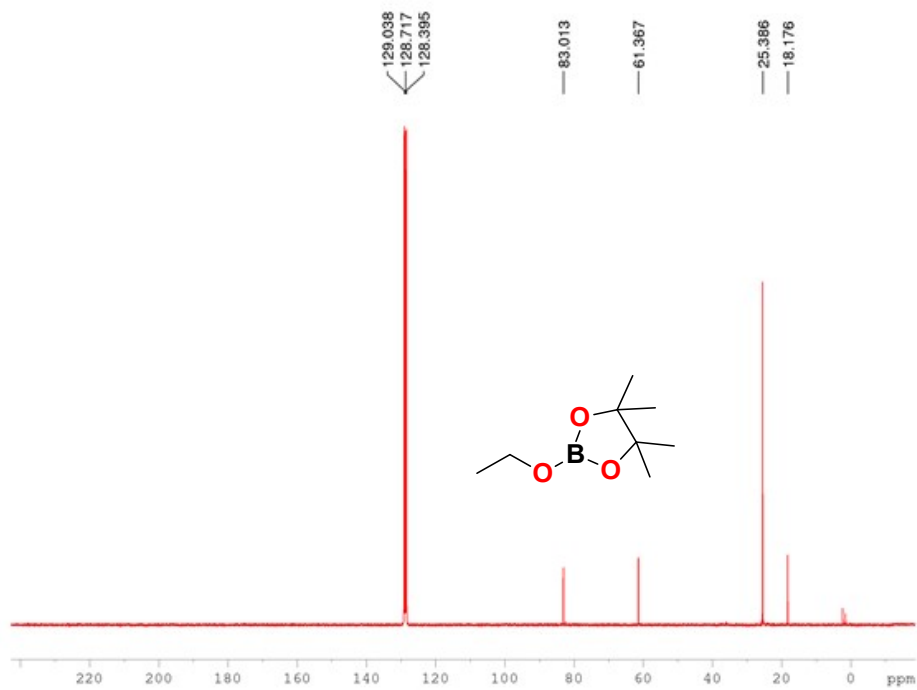


Figure S63. ^{13}C NMR spectrum (100 MHz, 25°C, C_6D_6) of compound **2 x 3r**.

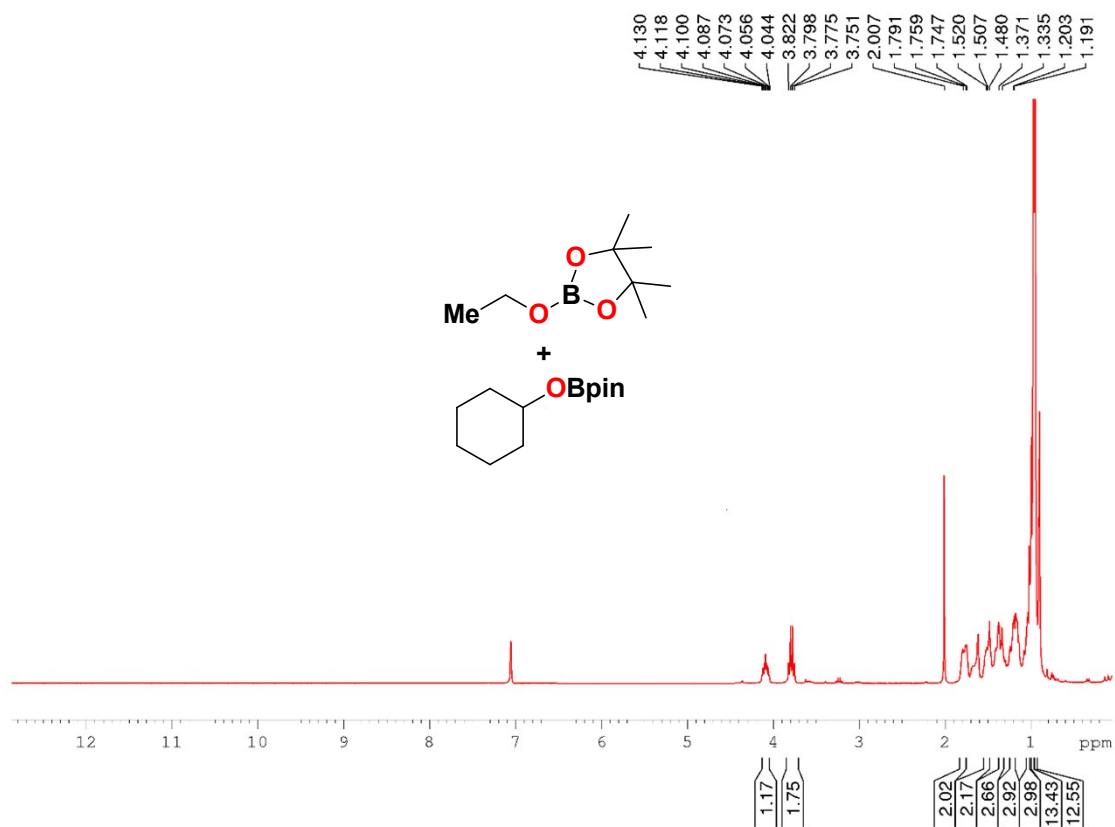


Figure S64. ¹H NMR spectrum (400 MHz, 25°C, C₆D₆) of compound 3r and 3s.

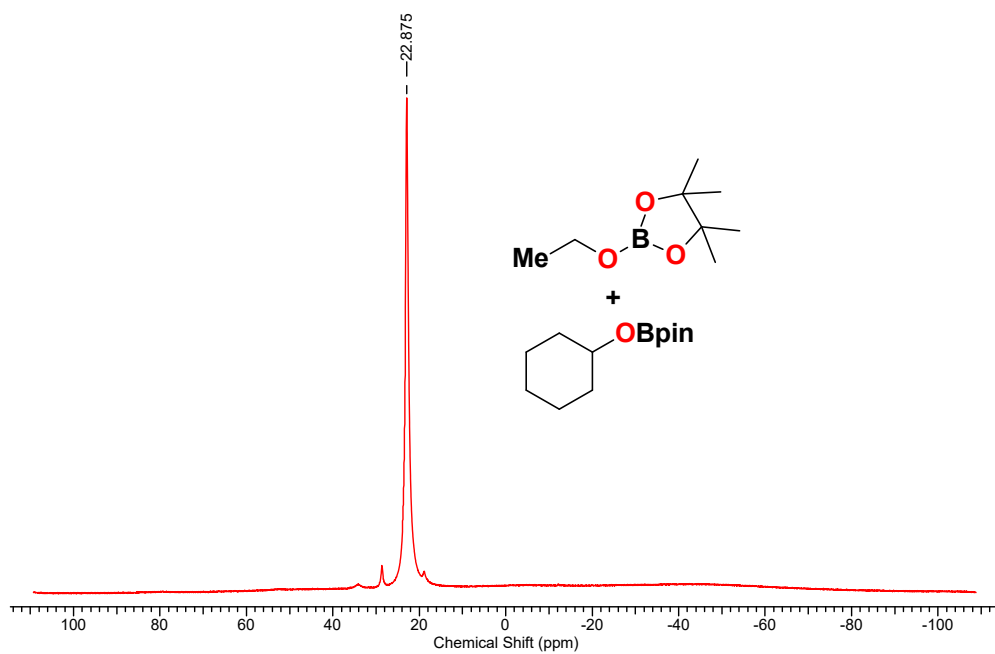


Figure S65. ¹¹B NMR spectrum (128.4 MHz, 25°C, C₆D₆) of compound 3r and 3s.

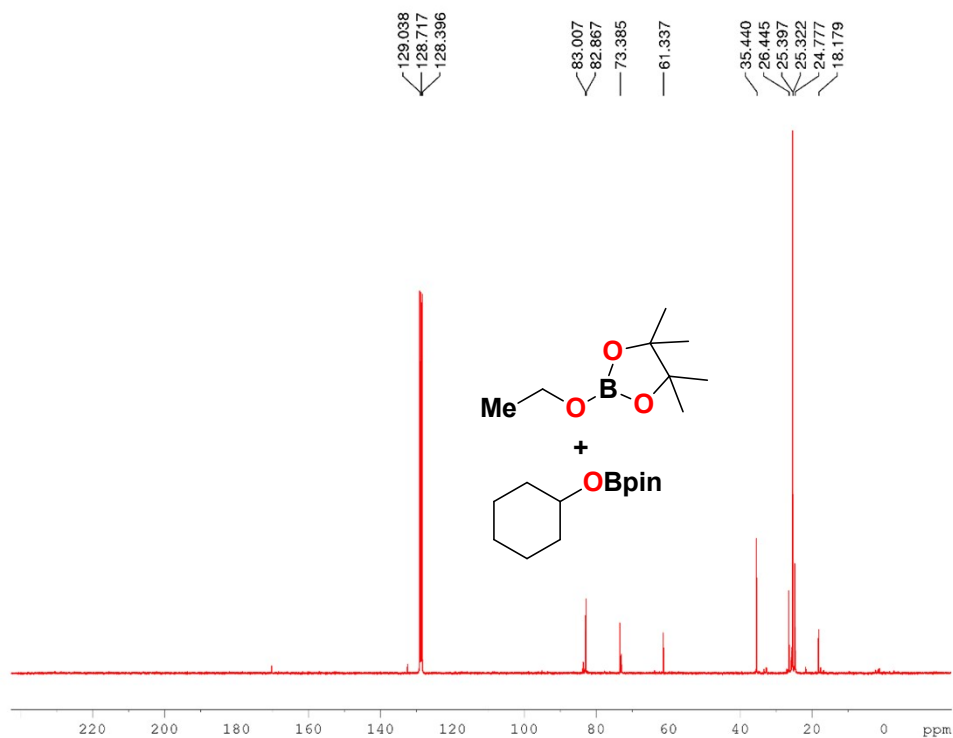


Figure S66. ^{13}C NMR spectrum (100 MHz, 25°C , C_6D_6) of compound **3r** and **3s**.

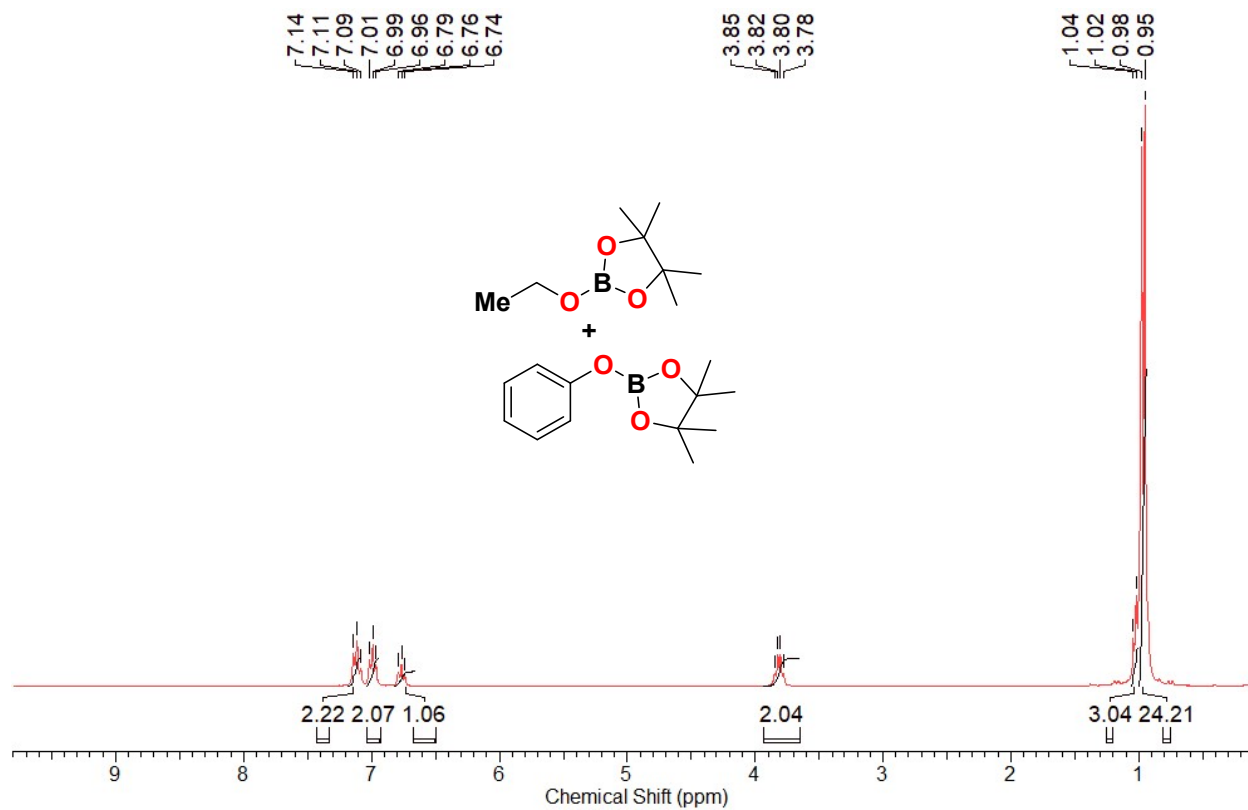


Figure S67. ^1H NMR spectrum (400 MHz, 25°C , C_6D_6) of compound **3r** and **3t**.

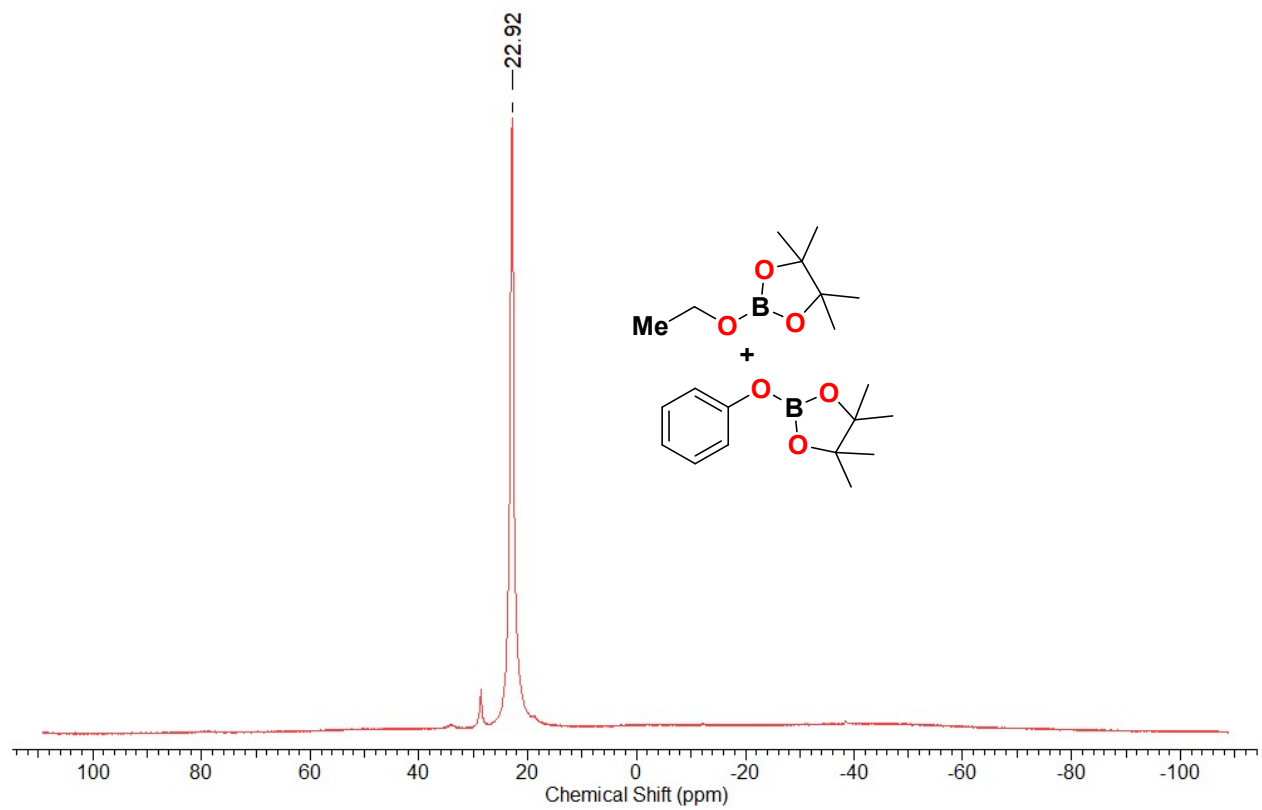


Figure S68. ^{11}B NMR spectrum (128.4 MHz, 25°C, C_6D_6) of compound **3r** and **3t**.

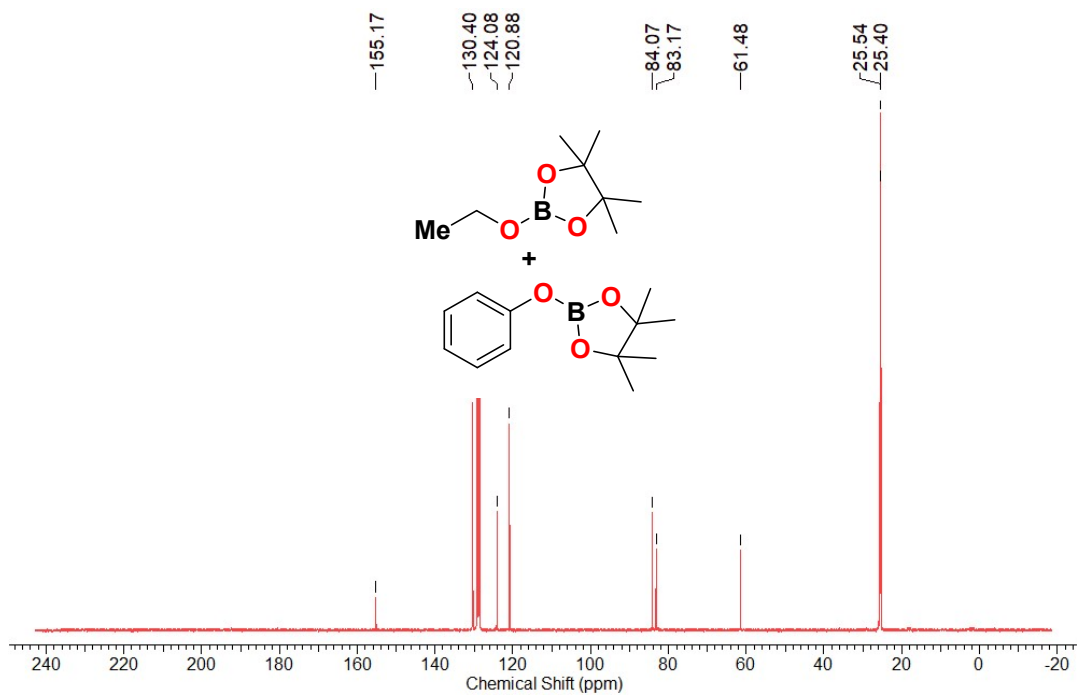


Figure S69. ^{13}C NMR spectrum (100 MHz, 25°C, C_6D_6) of compound **3r** and **3t**.

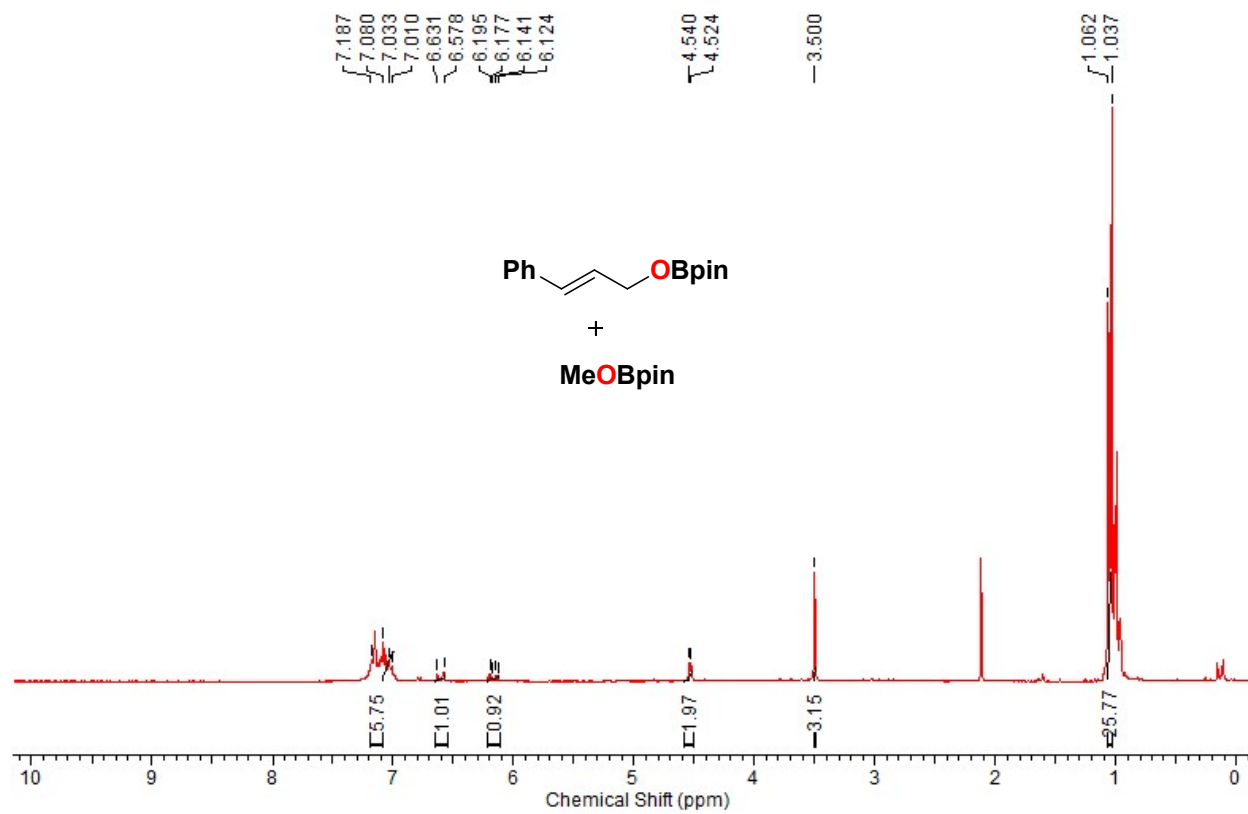


Figure S70. ^1H NMR spectrum (400 MHz, 25°C, C_6D_6) of compound **3u** and **3b**.

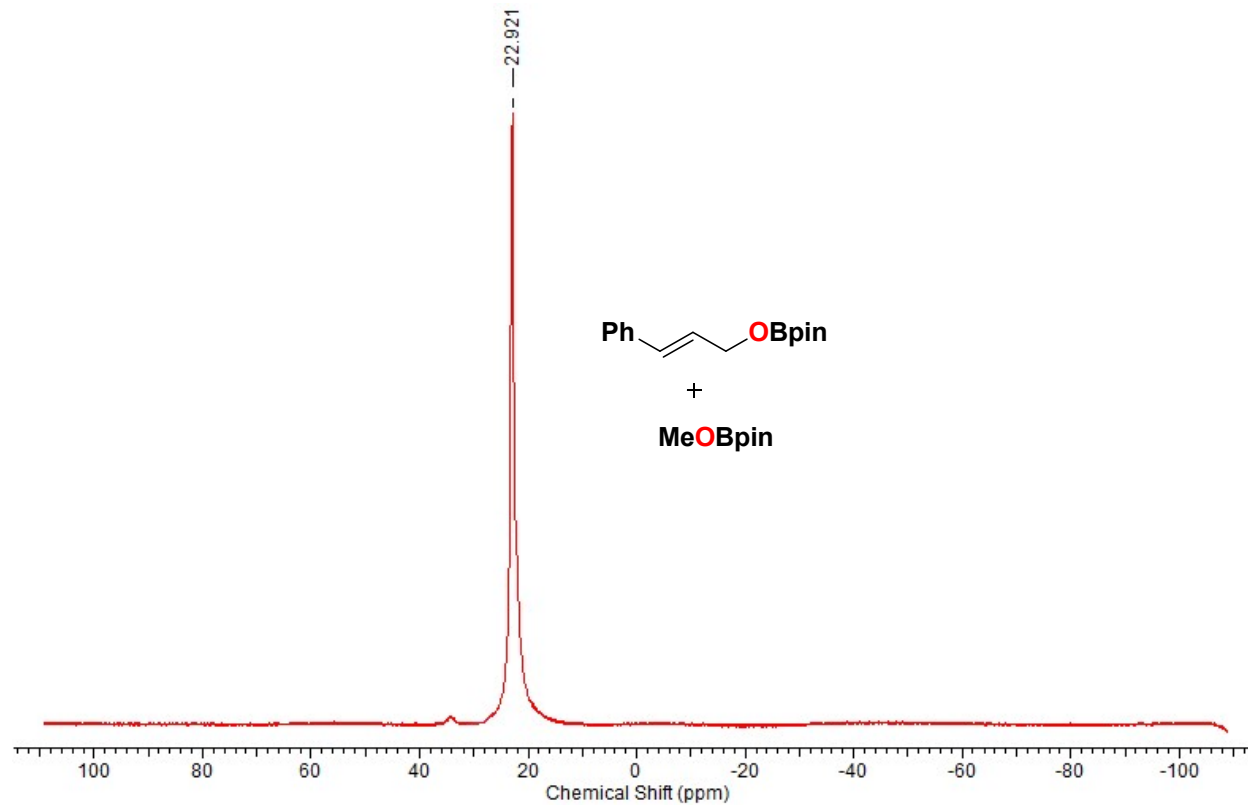


Figure S71. ^{11}B NMR spectrum (128.4 MHz, 25°C, C_6D_6) of compound **3u** and **3b**.

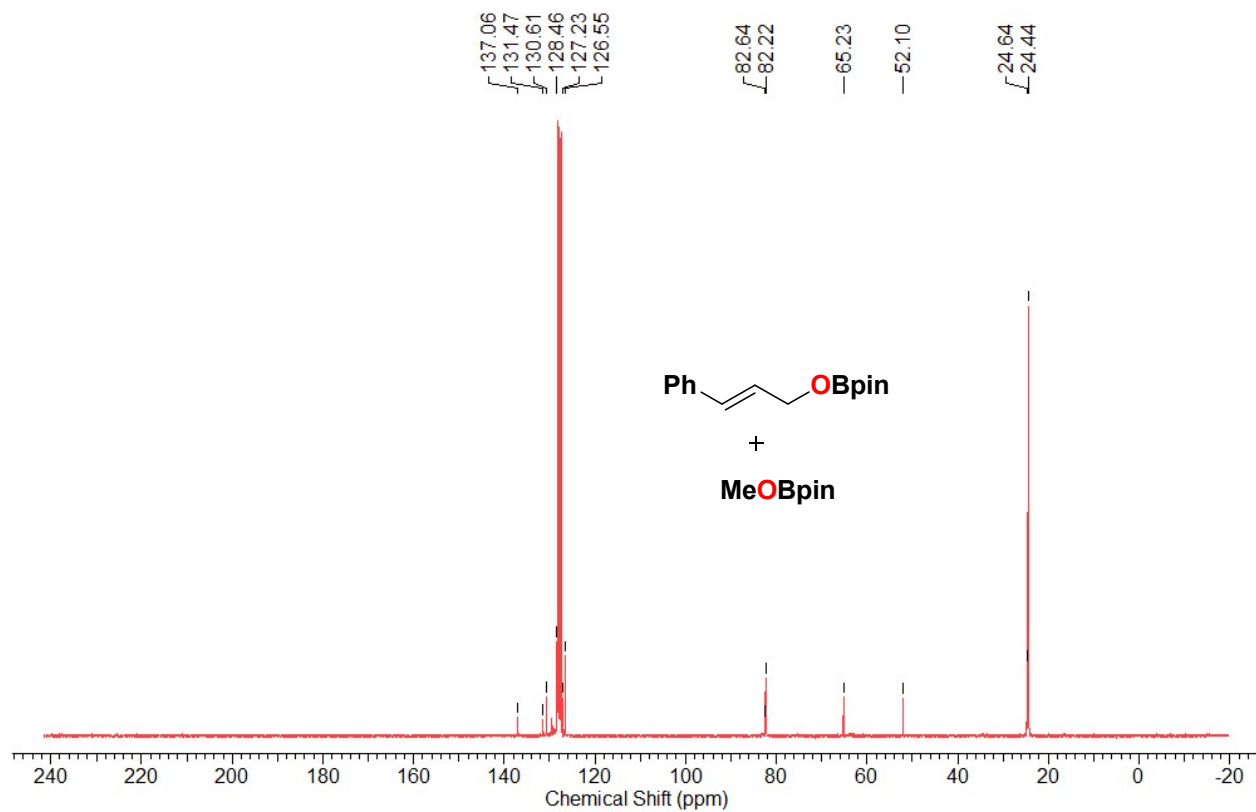


Figure S72. ^{13}C NMR spectrum (100 MHz, 25°C , C_6D_6) of compound **3u** and **3b**.

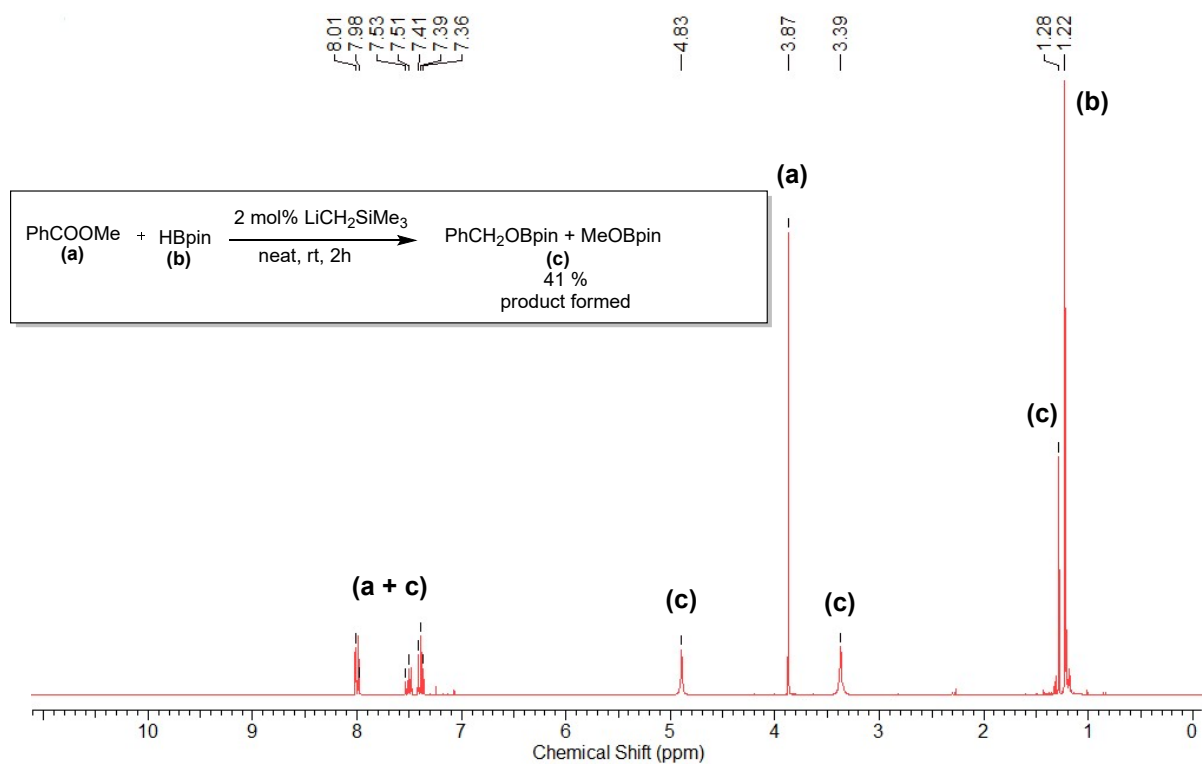


Figure S73. ^1H NMR spectrum (400 MHz, 25°C , C_6D_6) of the reaction PhCOOMe with HBpin catalyzed by $\text{LiCH}_2\text{SiMe}_3$.

(S6) Control Experiments:

HBPin + Complex 1 (1:1)

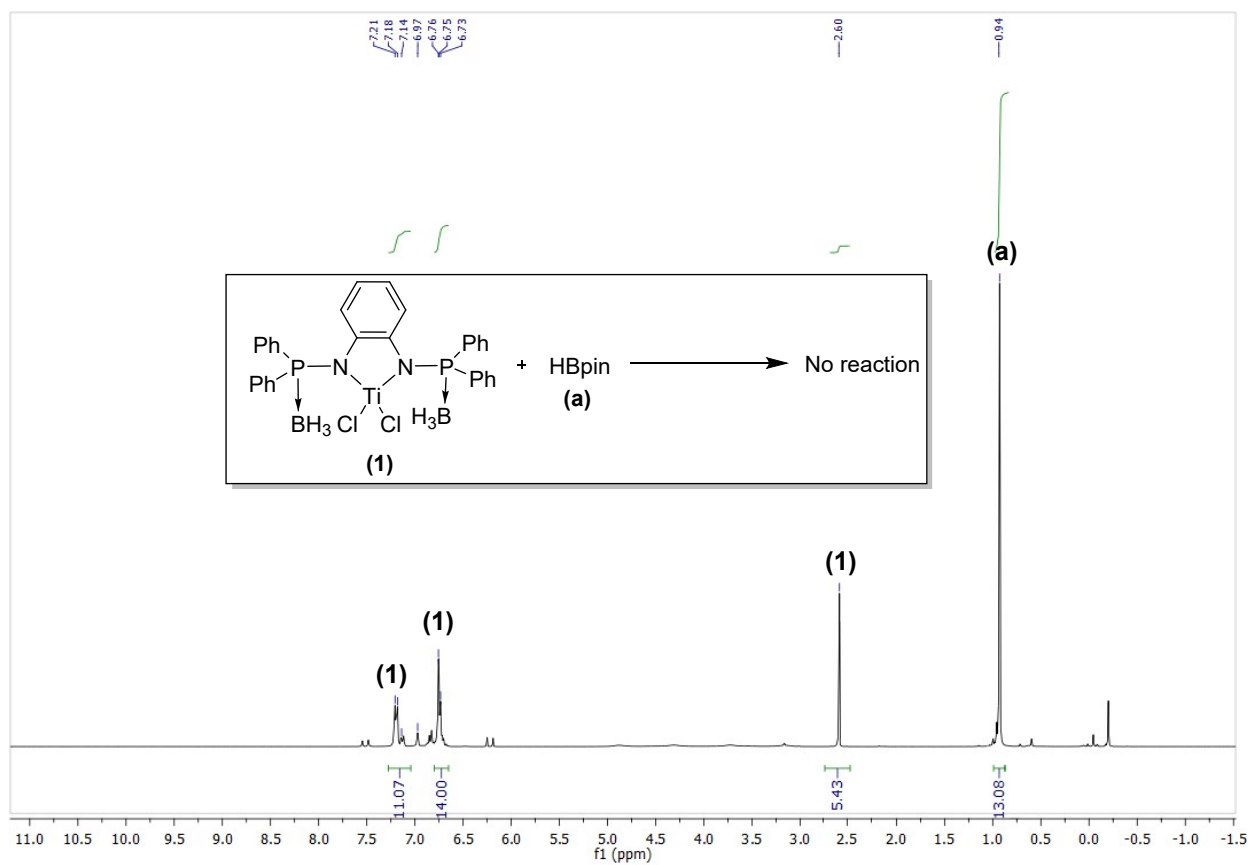


Figure S74. ^1H NMR spectrum (400 MHz, 25°C , C_6D_6) of the reaction of complex **1** with HBpin (1:1).

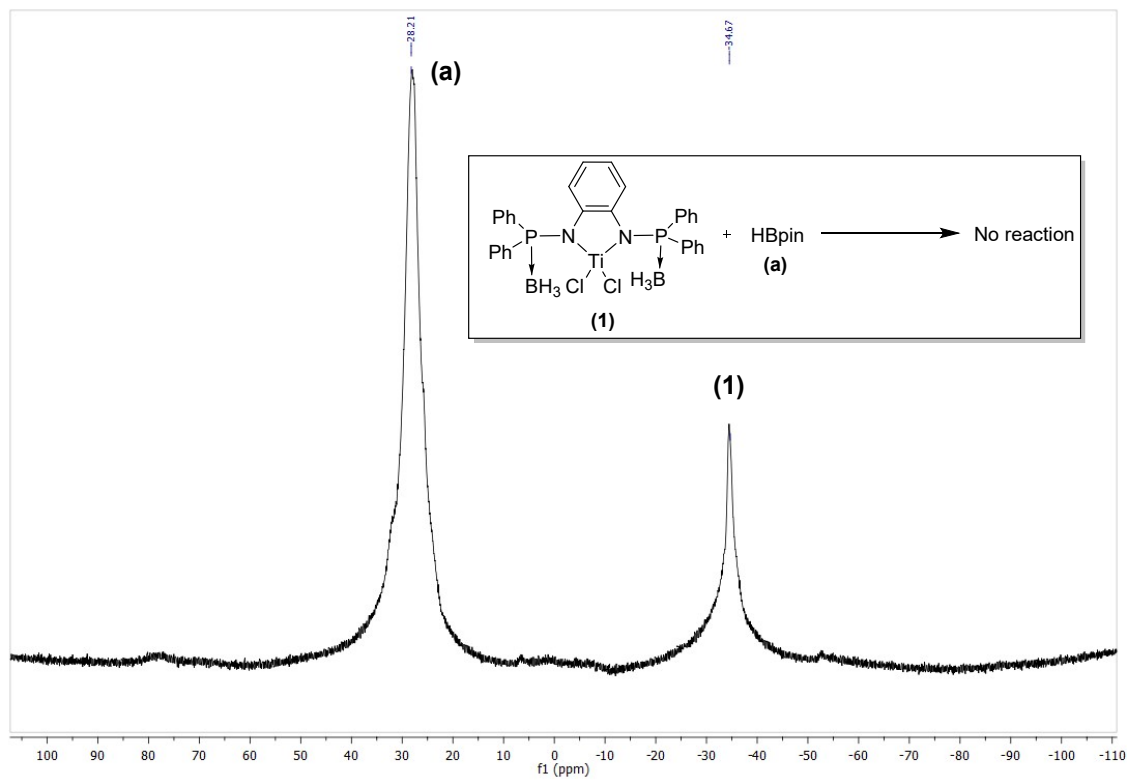


Figure S75. $^{11}\text{B}\{^1\text{H}\}$ NMR spectrum (128.4 MHz, 25°C, C_6D_6) of the reaction of complex **1** with HBpin (1:1).

HBpin + Complex 2 (1:1)

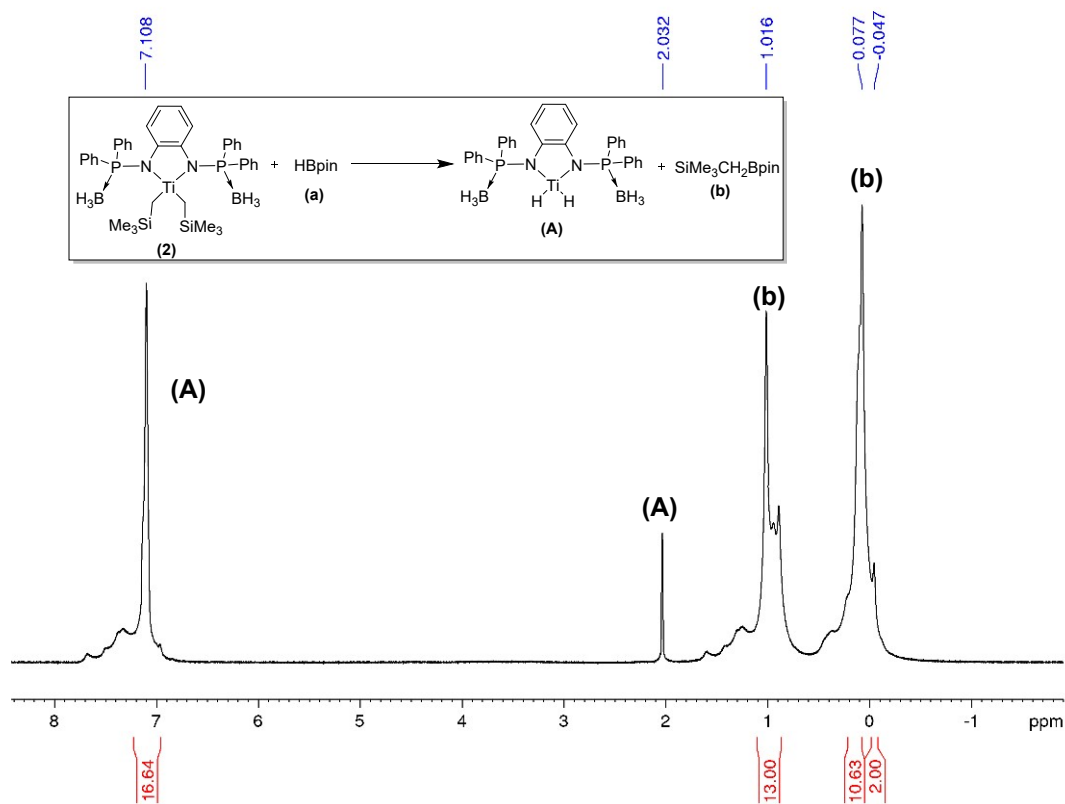


Figure S76. ^1H NMR spectrum (400 MHz, 25°C, C_6D_6) of the reaction of complex 2 with HBpin (1:1).

The NMR spectrum for the $\text{TiH}_2\text{C}_6\text{H}_4(\text{NPPh}_2\text{BH}_3)_2$ complex and $\text{CH}_2\text{SiMe}_3\text{Bpin}$ species (Figure S129-130). We failed to isolate a very clear NMR spectrum. The peaks that refer to Ti-H is not visible but the peaks that refer to $\text{CH}_2\text{SiMe}_3\text{Bpin}$ species are visible in both spectrum.

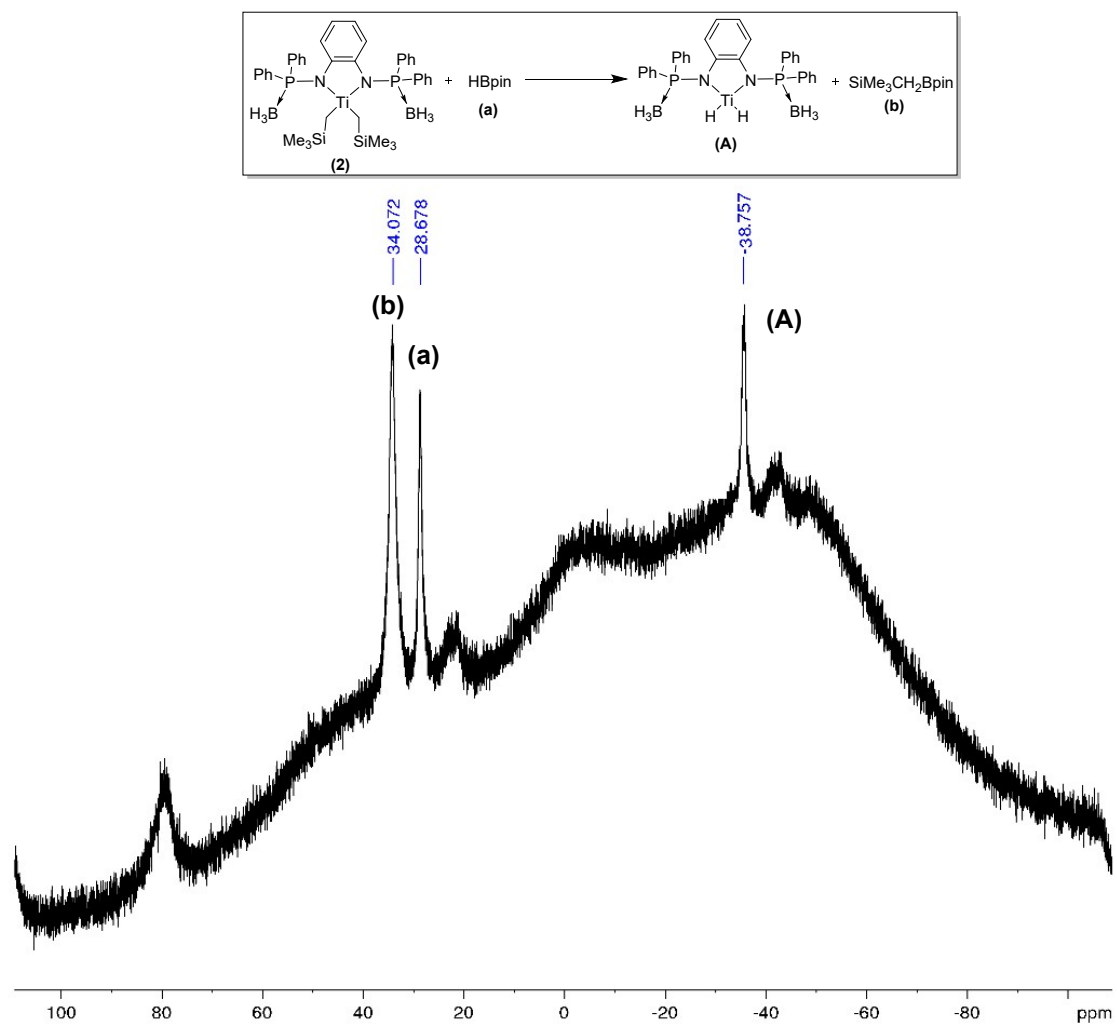


Figure S77. $^{11}\text{B}\{^1\text{H}\}$ NMR spectrum (128.4 MHz, 25°C, C_6D_6) of the reaction of complex **2** with HBpin (1:1).

Complex 2 + Ester (1:1)

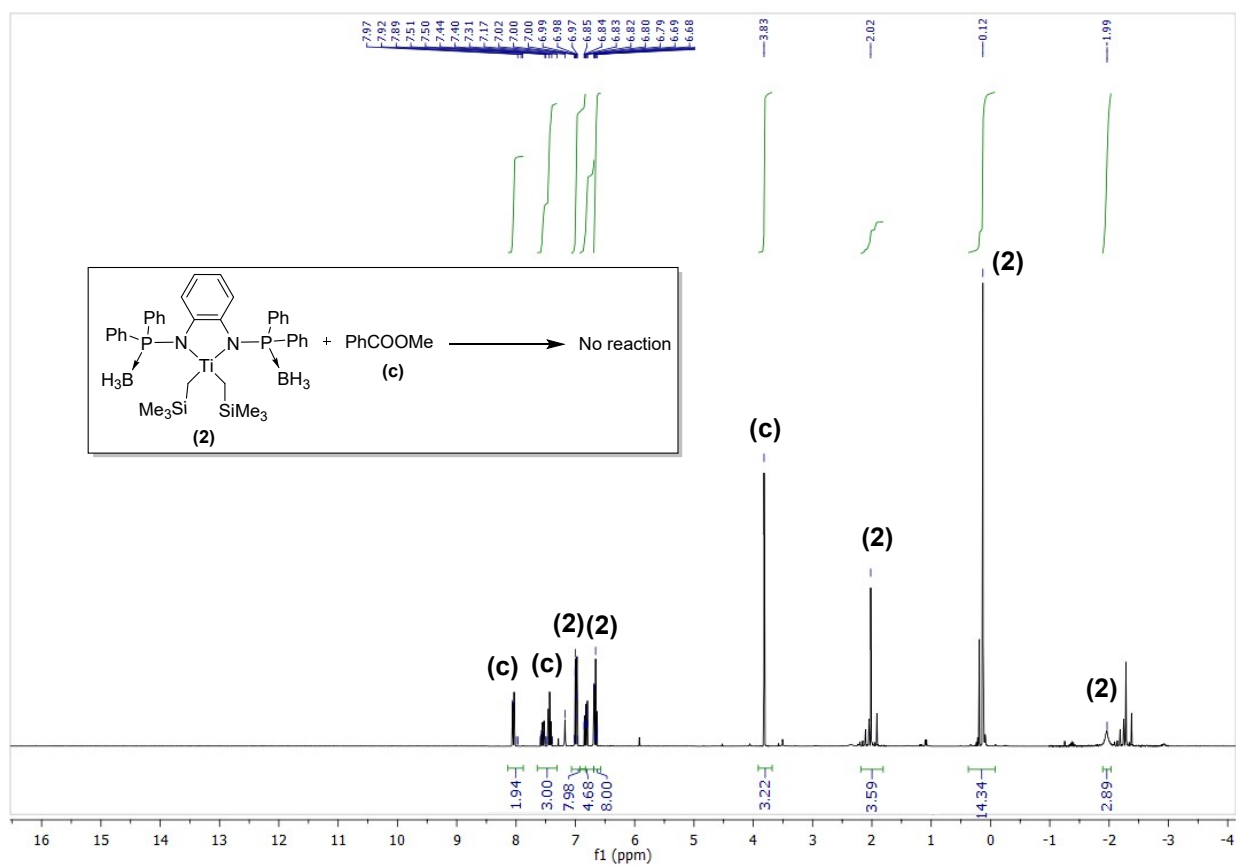


Figure S78. ^1H NMR spectrum (400 MHz, 25°C, C_6D_6) of the reaction of complex 2 with PhCOOMe (1:1).

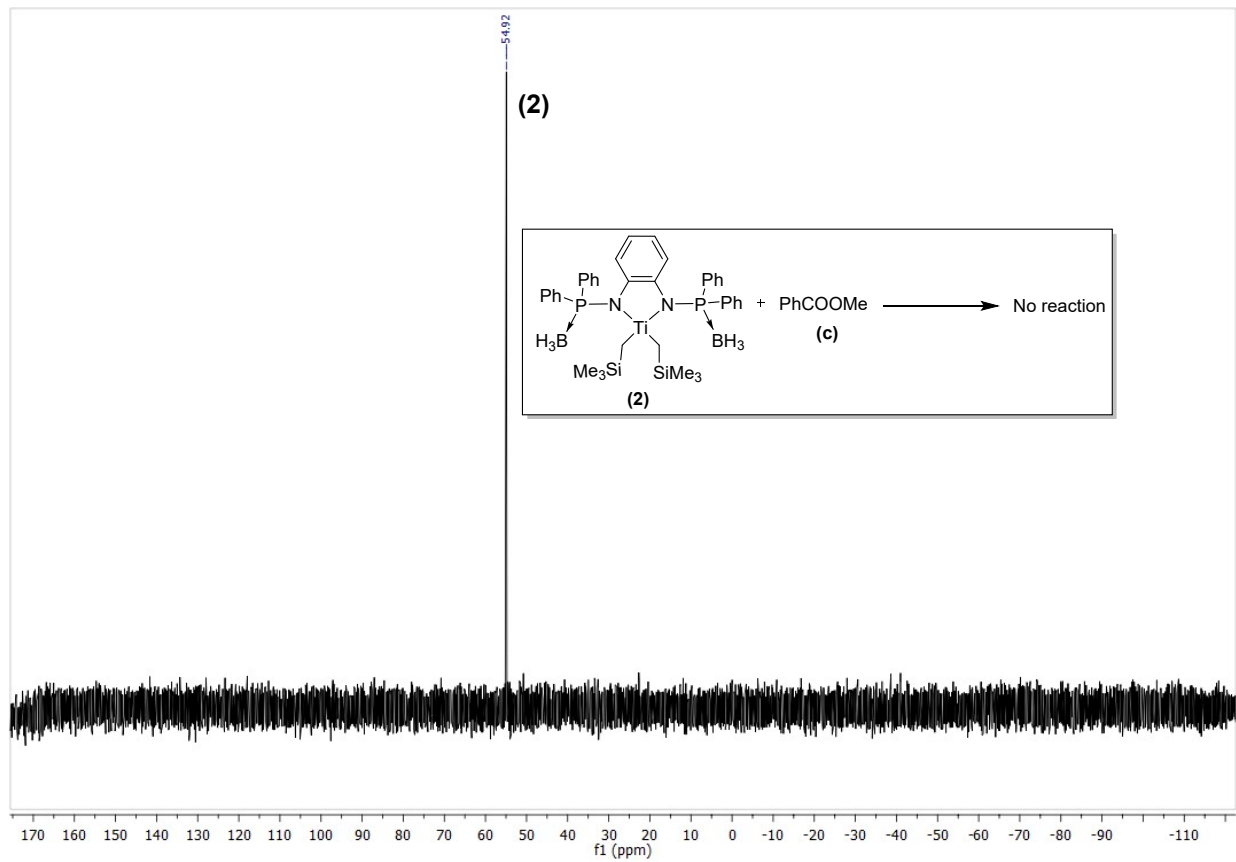


Figure S79. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum (161.9 MHz, 25°C, C_6D_6) of the reaction of complex **2** with PhCOOMe (1:1).

Complex 2 + Ester (1:1)

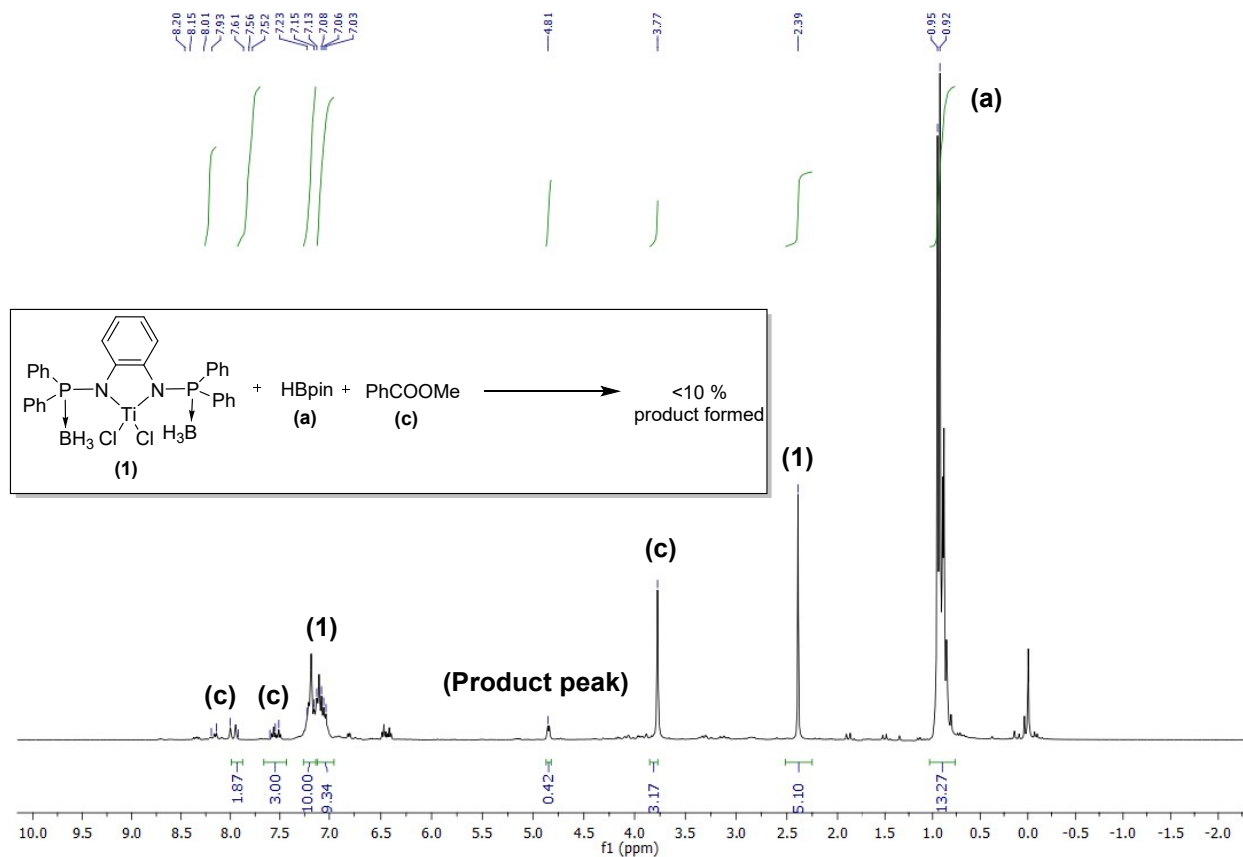


Figure S80. ¹H NMR spectrum (400 MHz, 25°C, C₆D₆) of the reaction of complex **1** with PhCOOMe and HBpin (1:1:1).

(S7) Kinetic analysis details:

Typical NMR-Scale Reaction for determining Kinetic Study by ¹H-NMR Arrays.

Kinetic Analysis. Kinetic analysis of the NMR-scale reactions described above was carried out by collecting multiple (>20) data points. The product concentration was measured from the area of the PhCH₂OBpin peak formed with respect to their starting material peak standardized to the methyl peak area of the C₆Me₆ internal standard. The order of the catalyst and each substrate was determined from the linearity of plots of [product] vs. time (zeroth order), ln[product] vs. time (first-order), and [product]⁻¹ vs. time (second-order) having R² value close towards 1.

[Catalyst] rate order assessment

In a glove box, the respective amount of complex **2** (0.010, 0.015, 0.02, 0.025, 0.03 M), PhCOOMe (0.060g, 0.5 mmol) and HBpin (0.128 g, 1.0 mmol), and the internal standard, hexamethylbenzene (8 mg, 0.05 M), was added in a vial and after that C₆D₆ (1 mL) was added to these reaction mixture. From this stock solution finally, 0.5 mL aliquot were taken out and it was added to a rubber septum-sealed NMR tube, wrapped with parafilm, and removed from the

box. The solution was set in the NMR tube at 25 °C. After that, the tube was shaken and reinserted into the instrument again and scanning was begun. Single (¹H NMR) scans were collected at regular intervals.

Varying concentration of catalyst (10–30 mM), keeping HBPin (1.0 M) and methylbenzoate (0.5 M) concentration constant, which follows first-order dependence with respect to [catalyst] (Figure S75–S76).

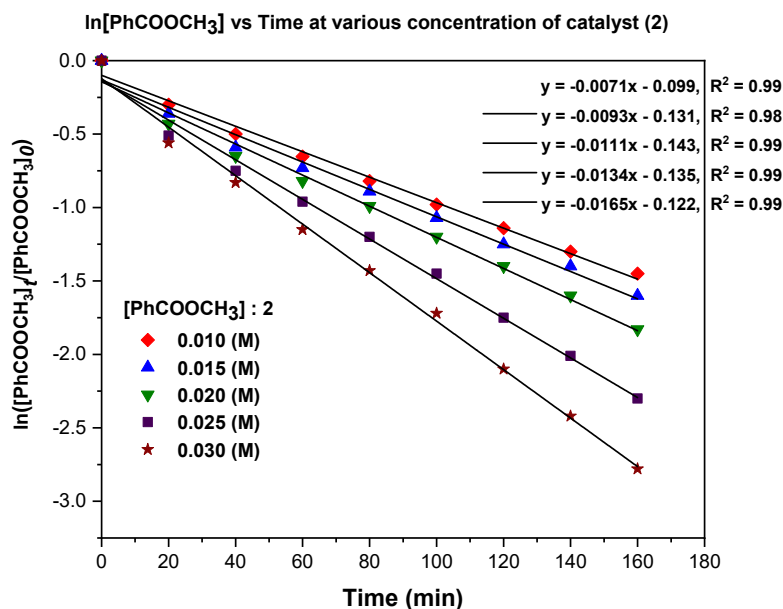


Figure S81. First order kinetic plots for ester hydroboration reaction in C₆D₆ (1 mL) with different concentrations of [(CH₂SiMe₃)₂Ti{Ph₂P(BH₃)N}₂C₆H₄] (**2**) at 25 °C. Reaction conditions: [HBPin] = 1.0 M and [PhCOOCH₃] = 0.5 M, [(CH₂SiMe₃)₂Ti{Ph₂P(BH₃)N}₂C₆H₄] = (10–30 mM) in C₆D₆ (total volume 1 mL).

Table S2. Data for kinetic plot of *k*_{obs} (obtained from first order kinetics plots) vs [(CH₂SiMe₃)₂Ti{Ph₂P(BH₃)N}₂C₆H₄] for the ester hydroboration reaction of PhCOOCH₃ with HBPin in presence of catalyst (**2**). Reaction conditions: [HBPin] = 1.0 M and [PhCOOCH₃] = 0.5 M, [(CH₂SiMe₃)₂Ti{Ph₂P(BH₃)N}₂C₆H₄] = (10–30 mM) in C₆D₆ (1 mL).

S.NO.	[2]	<i>k</i> _{obs} (min ⁻¹)
1	0.010	0.007
2	0.015	0.009
3	0.02	0.011
4	0.025	0.013
5	0.03	0.016

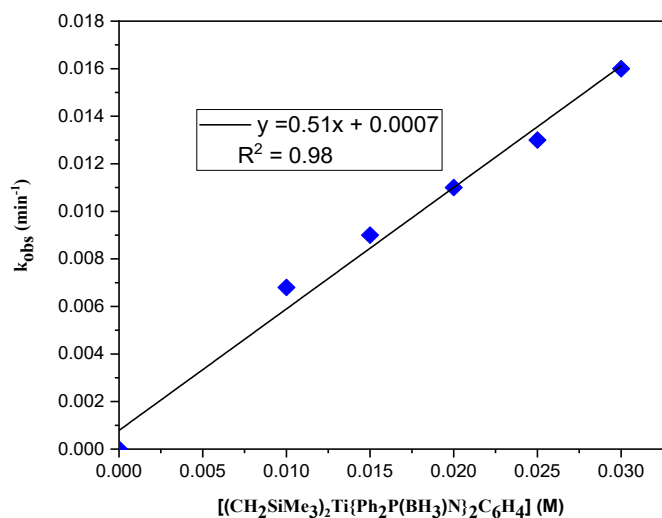
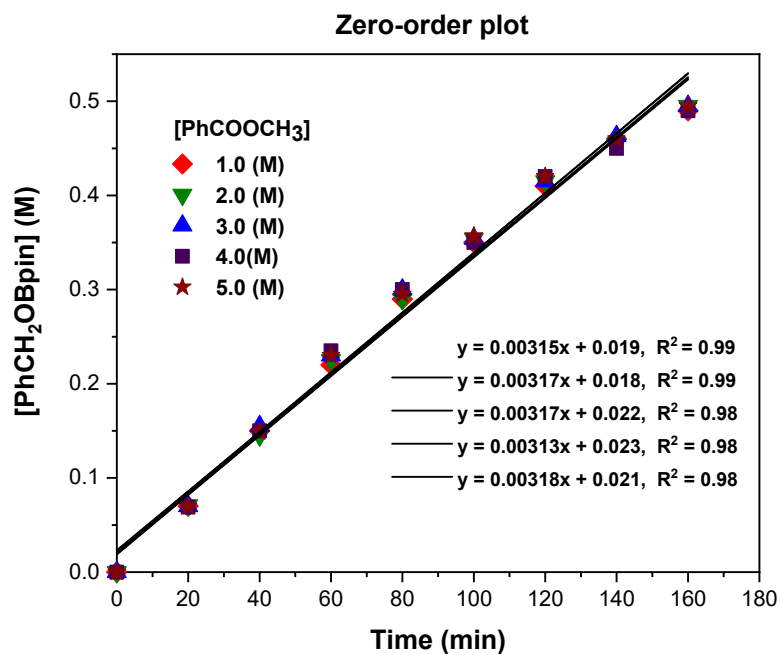


Figure S82. Kinetics plot of k_{obs} vs $[(\text{CH}_2\text{SiMe}_3)_2\text{Ti}\{\text{Ph}_2\text{P}(\text{BH}_3)\text{N}\}_2\text{C}_6\text{H}_4]$ for ester hydroboration reaction in C_6D_6 (1 mL) at 25 °C. Reaction conditions: $[\text{HBpin}] = 1.0 \text{ M}$ and $[\text{PhCOOCH}_3] = 0.5 \text{ M}$, $[(\text{CH}_2\text{SiMe}_3)_2\text{Ti}\{\text{Ph}_2\text{P}(\text{BH}_3)\text{N}\}_2\text{C}_6\text{H}_4] = (10\text{--}30 \text{ mM})$ in C_6D_6 (1.0 mL). The order of catalyst = 1.

[Ester] rate order assessment

Varying concentration of methylbenzoate (1.0–5.0 M), keeping HBpin (1.0 M) and catalyst (15 mM) concentration constant, which follows zero-order dependence with respect to $[\text{PhCOOCH}_3]$ (Figure S77–S78).



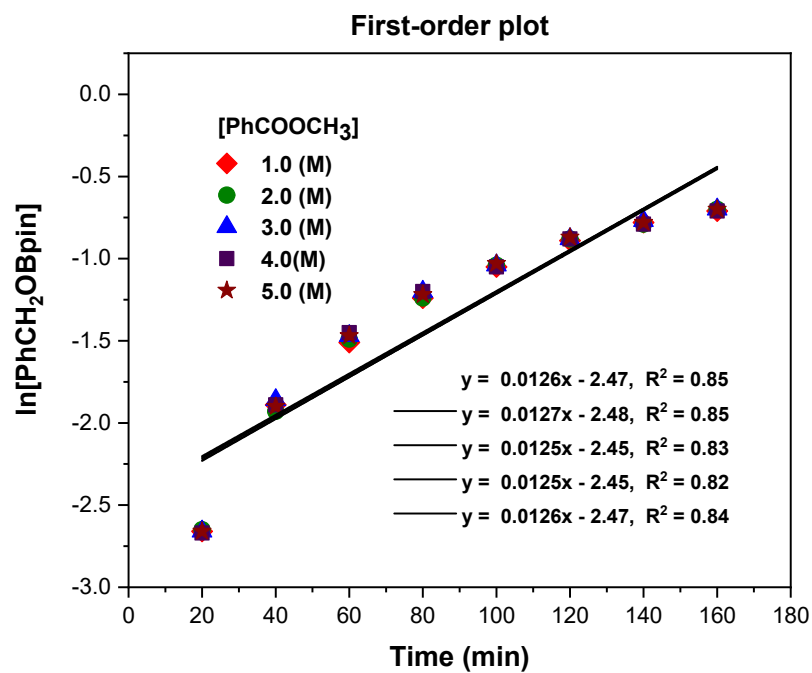


Figure S83. Different order kinetics plots for ester hydroboration reaction in C_6D_6 (1 mL) at 25 °C. Reaction conditions: $[HBPin] = 1.0$ M and $[PhCOOCH_3] = (1.0-5.0)$ M, $[(CH_2SiMe_3)_2Ti\{Ph_2P(BH_3)N\}_2C_6H_4] = 15$ mM in C_6D_6 (1.0 mL). Only the zeroth-order plots are linear with R^2 value close to 1 while the other two plots are nonlinear.

Table S3. Data for kinetic plot of k_{obs} vs $[\text{PhCOOCH}_3]$ (obtained from zero order kinetics plots) for the ester hydroboration reaction of PhCOOCH_3 with HBPin in presence of catalyst **2**. Reaction conditions: $[(\text{CH}_2\text{SiMe}_3)_2\text{Ti}\{\text{Ph}_2\text{P}(\text{BH}_3)\text{N}\}_2\text{C}_6\text{H}_4] = 15 \text{ mM}$, $[\text{HBpin}] = 1.0 \text{ M}$ and $[\text{PhCOOCH}_3] = (1.0\text{--}5.0 \text{ M})$ in C_6D_6 (1.0 mL).

S.NO.	$[\text{PhCOOCH}_3]$	k_{obs} (Mmin ⁻¹)
1	1.0	0.00315
2	2.0	0.00317
3	3.0	0.00317
4	4.0	0.00313
5	5.0	0.00318

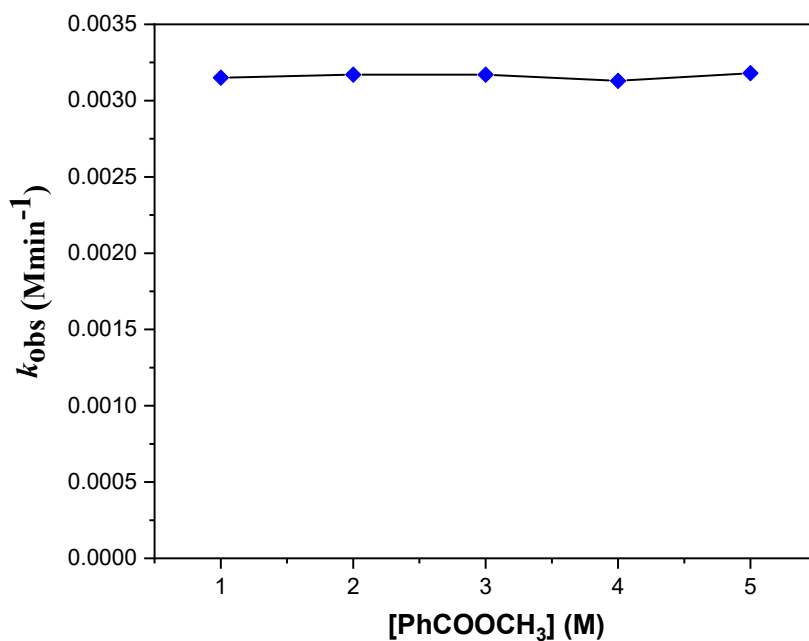
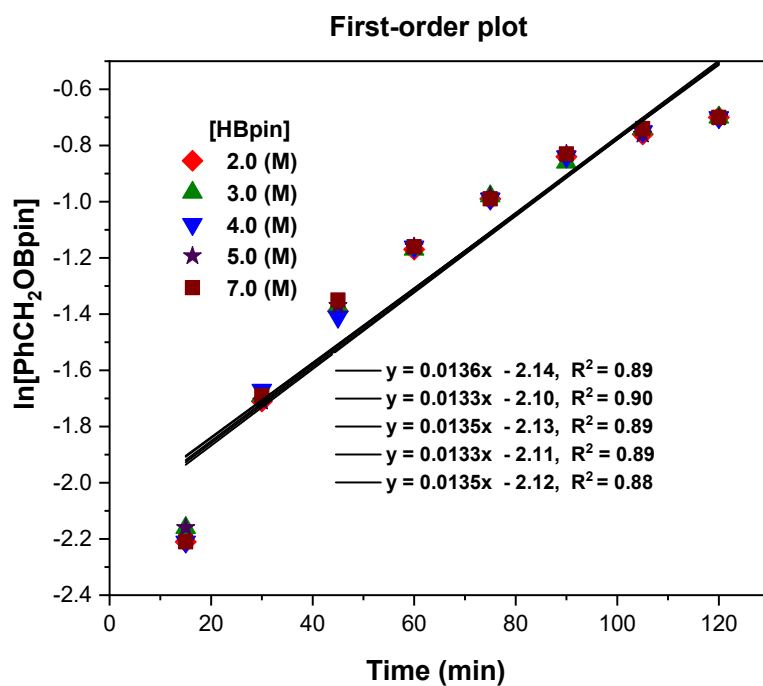
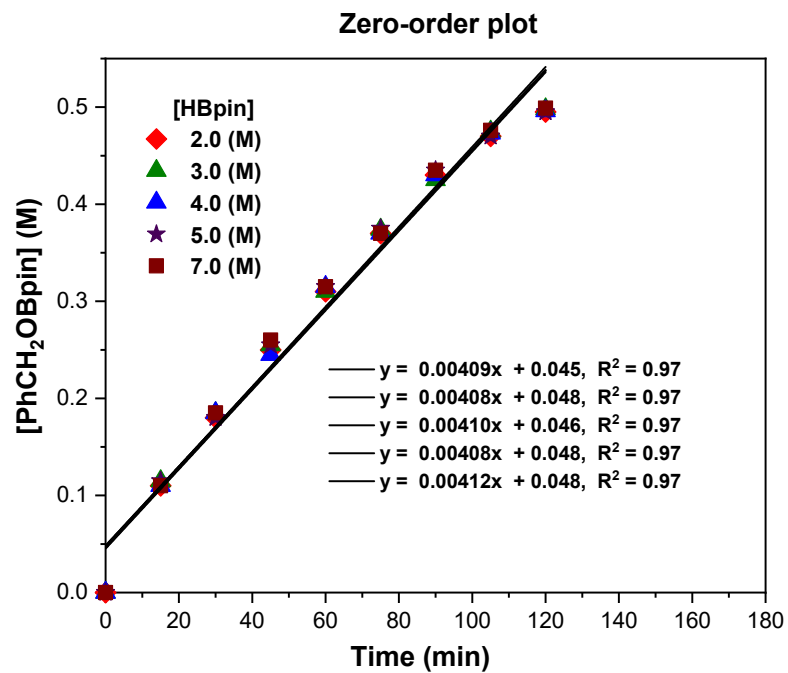


Figure S84. Kinetics plot of k_{obs} vs $[\text{PhCOOCH}_3]$ for ester hydroboration reaction in C_6D_6 (1 mL) at 25 °C. Reaction conditions: $[\text{HBpin}] = 1.0 \text{ M}$ and $[\text{PhCOOCH}_3] = (1.0\text{--}5.0 \text{ M})$, $[(\text{CH}_2\text{SiMe}_3)_2\text{Ti}\{\text{Ph}_2\text{P}(\text{BH}_3)\text{N}\}_2\text{C}_6\text{H}_4] = 15 \text{ mM}$ in C_6D_6 (1.0 mL). The order of $\text{PhCOOCH}_3 = 0$ (slope = 0.0002 \approx 0).

[HBpin] rate order assessment

Varying concentration of HBpin (2.0–7.0 M), keeping methylbenzoate (0.5 M) and catalyst (15 mM) concentration constant, which follows zero-order dependence with respect to [HBpin] (Figure S79–S80).



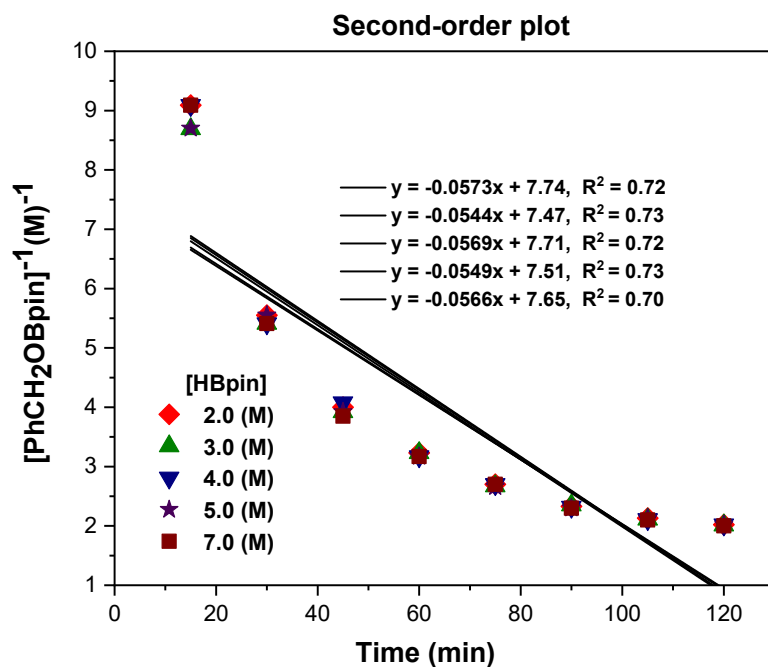


Figure S85. Different order kinetics plots for ester hydroboration reaction in C_6D_6 (1 mL) at 25 °C. Reaction conditions: $[HBpin] = (2.0-7.0)$ M and $[PhCOOCH_3] = 0.5$ M, $[(CH_2SiMe_3)_2Ti\{Ph_2P(BH_3)N\}_2C_6H_4] = 15$ mM in C_6D_6 (1.0 mL). Only the zeroth-order plots are linear with R^2 value close to 1 while the other two plots are nonlinear.

Table S4. Data for kinetic plot of k_{obs} vs $[HBpin]$ (obtained from zero order kinetics plots) for the ester hydroboration reaction of $PhCOOCH_3$ with $HBpin$ in presence of catalyst **2**. Reaction conditions: $[(CH_2SiMe_3)_2Ti\{Ph_2P(BH_3)N\}_2C_6H_4] = 15$ mM, $[HBpin] = (2.0-7.0)$ M and $[PhCOOCH_3] = 0.5$ M in C_6D_6 (1.0 mL).

S.NO.	$[HBpin]$	$k_{obs} (Mmin)^{-1}$
1	2.0	0.00409
2	3.0	0.00408
3	4.0	0.00410
4	5.0	0.00408
5	7.0	0.00412

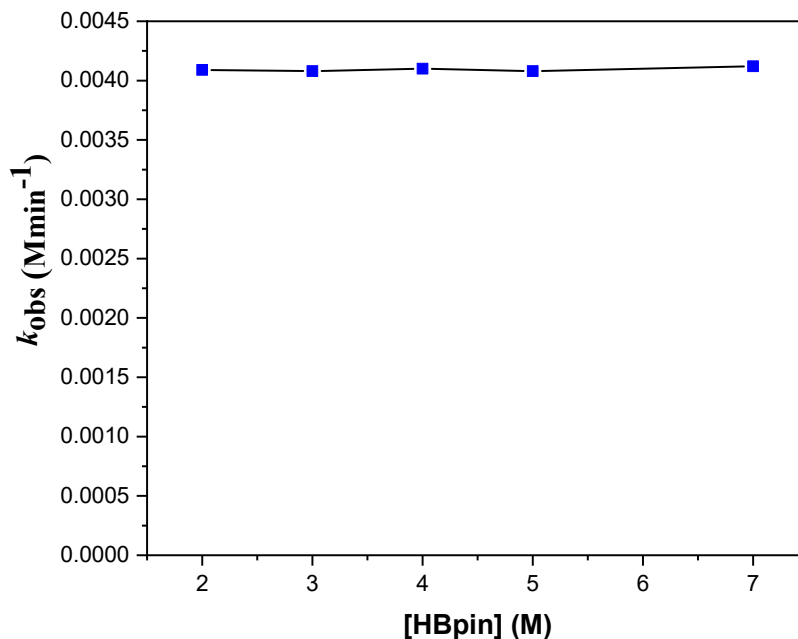


Figure S86. Kinetics plot of k_{obs} vs [HBpin] for ester hydroboration reaction in C_6D_6 (1 mL) at 25 °C. Reaction conditions: [HBpin] = (2.0–7.0) M and [PhCOOCH₃] = 0.5 M, [(CH₂SiMe₃)₂Ti{Ph₂P(BH₃)N}₂C₆H₄} = 15 mM in C_6D_6 (1.0 mL). The order of PhCOOCH₃ = 0 (slope = 0.0009 ≈ 0).

Eyring/Arrhenius plots:

Temperature-dependent rate data were obtained *via* arrayed NMR measurement as described above. Temperatures were set on the NMR instrument using an external temperature controller and calibrated using ethylene glycol (>25 °C) or methanol (<25 °C) standards. Rates at each temperature were determined from the average of five trials.

These data were then plotted as $1/T$ vs. $\ln(k/T)$ from which the enthalpy and entropy of the transition state could be obtained using the Eyring equation (see eq. A). ΔH^\ddagger is the negative slope times R and ΔS^\ddagger is the intercept minus the natural log of k_b/h times R. (Figure 82)

$$\ln \frac{k}{T} = \frac{-\Delta H^\ddagger}{R} \cdot \frac{1}{T} + \ln \frac{k_B}{h} + \frac{\Delta S^\ddagger}{R} \text{ -----Eq (A)}$$

From a plot of $1/T$ vs. $\ln(k)$, the activation energy can be obtained using the Arrhenius equation (eq. B). E_a is the negative slope times R. (Figure 83)

$$\ln k = -\frac{E_a}{RT} + \ln A \text{ -----Eq (B)}$$

The activation parameters for the Hydroboration of ester with Pinacolborane catalyzed by $[(\text{CH}_2\text{SiMe}_3)_2\text{Ti}\{\text{Ph}_2\text{P}(\text{BH}_3)\text{N}\}_2\text{C}_6\text{H}_4]$ (**2**) in C_6D_6 were found to be ΔH^\ddagger 2.52(1) kcal.mol⁻¹ and ΔS^\ddagger -40.36 (3) cal/(mol.K), ΔE_a = 3.3(1) kcal.mol⁻¹. A ΔG^\ddagger value of 14.55 kcal.mol⁻¹ was calculated for the Hydroboration of esters with Pinacolborane by the titanium alkyl catalyst (**2**) at 25 °C.

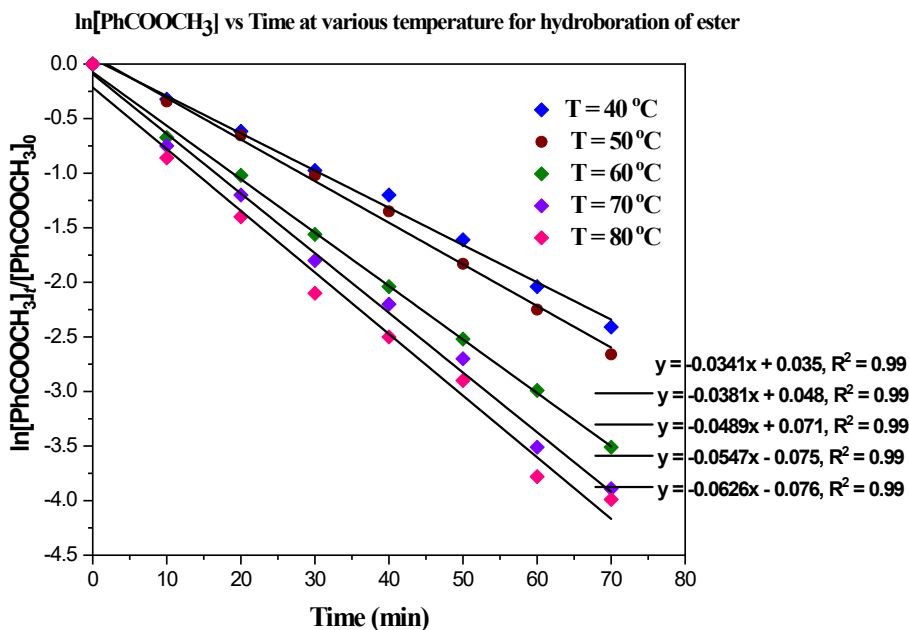


Figure S87. First order kinetic plots for hydroboration reaction of PhCOOCH_3 in C_6D_6 (1 mL) at different temperatures using catalyst $[(\text{CH}_2\text{SiMe}_3)_2\text{Ti}\{\text{Ph}_2\text{P}(\text{BH}_3)\text{N}\}_2\text{C}_6\text{H}_4]$ (**2**). Reaction conditions: $[\text{HBPin}] = 1.0$ M and $[\text{PhCOOCH}_3] = 0.5$ M, $[(\text{CH}_2\text{SiMe}_3)_2\text{Ti}\{\text{Ph}_2\text{P}(\text{BH}_3)\text{N}\}_2\text{C}_6\text{H}_4] = 15$ mM in C_6D_6 (1.0 mL).

Table S5. Data for Eyring and Arrhenius plots of $\ln(k_{\text{obs}}/T)$ vs $(1/T)$ and $\ln(k_{\text{obs}})$ vs $(1/T)$ catalyzed by $[(\text{CH}_2\text{SiMe}_3)_2\text{Ti}\{\text{Ph}_2\text{P}(\text{BH}_3)\text{N}\}_2\text{C}_6\text{H}_4]$ (**2**) [Reaction conditions: $[\text{HBPin}] = 1.0$ M and $[\text{PhCOOCH}_3] = 0.5$ M, $[(\text{CH}_2\text{SiMe}_3)_2\text{Ti}\{\text{Ph}_2\text{P}(\text{BH}_3)\text{N}\}_2\text{C}_6\text{H}_4] = 15$ mM in C_6D_6 (1.0 mL)].

S.NO.	T in K	(1/T) [K ⁻¹]	k_{obs} [min ⁻¹]	$\ln k_{\text{obs}}$	$\ln(k_{\text{obs}}/T)$
1	303	0.0033	0.0341(1)	-3.37	-9.09
2	313	0.00319	0.0381(1)	-3.27	-9.01
3	323	0.0031	0.0489(1)	-3.05	-8.79
4	328	0.003	0.0547(2)	-2.91	-8.69
5	338	0.0029	0.0626(3)	-2.77	-8.59

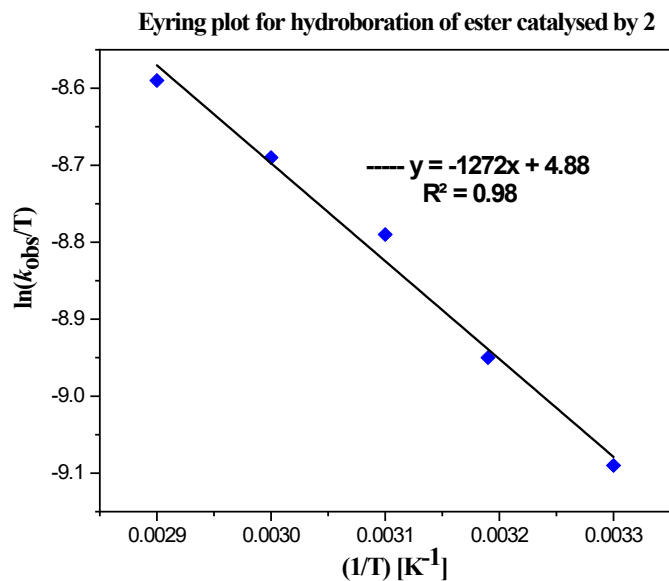


Figure S88. Eyring plot of $\ln(k_{\text{obs}}/T)$ vs $(1/T)$ for titanium alkyl (**2**) catalyzed hydroboration reaction of PhCOOCH_3 in C_6D_6 (1.0 mL) having $\Delta H^\ddagger = 2.52(1)$ kcal mol⁻¹ $\Delta S^\ddagger = -40.36$ (3) cal mol⁻¹K⁻¹. Reaction conditions: $[\text{HBPin}] = 1.0$ M and $[\text{PhCOOCH}_3] = 0.5$ M, $[(\text{CH}_2\text{SiMe}_3)_2\text{Ti}\{\text{Ph}_2\text{P}(\text{BH}_3)\text{N}\}_2\text{C}_6\text{H}_4] = 15$ mM in C_6D_6 (1.0 mL)

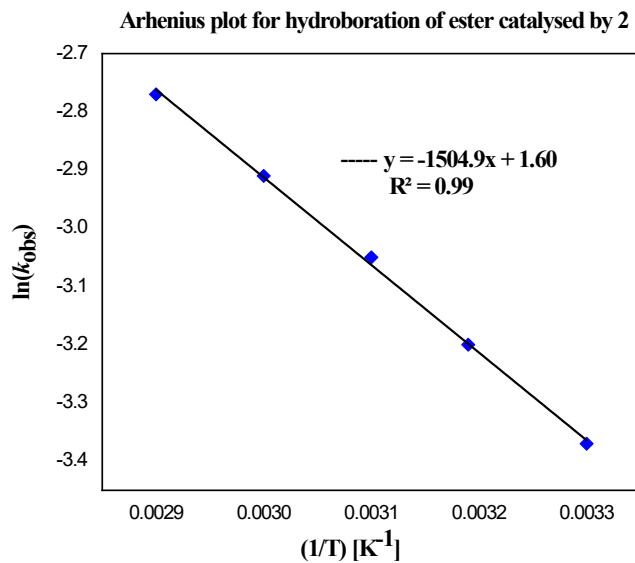


Figure S89. Arrhenius plot of $\ln(k_{\text{obs}}/T)$ vs $(1/T)$ for titanium alkyl (**2**) catalyzed hydroboration reaction of PhCOOCH_3 in C_6D_6 (0.4 mL) having $E_a = 3.3(1)$ kcal mol⁻¹. Reaction conditions: $[\text{HBPin}] = 1.0$ M and $[\text{PhCOOCH}_3] = 0.5$ M, $[(\text{CH}_2\text{SiMe}_3)_2\text{Ti}\{\text{Ph}_2\text{P}(\text{BH}_3)\text{N}\}_2\text{C}_6\text{H}_4] = 15$ mM in C_6D_6 (1.0 mL).

(S8) Computational Method:

All calculations were performed using the ORCA quantum chemical program package^[4]. Geometries were optimized with the GGA (generalized gradient approximation) density functional BP86^[5-6] in conjunction with def2-SVP^[7] basis sets. To accelerate the overall calculations, the RI^[8-10] (resolution-of-identity) approximation was applied for the expensive integral calculations. Noncovalent interactions were accounted by using atom-pairwise dispersion corrections with Becke-Johnson (D3BJ) damping.^[11] Subsequent numerical frequency calculations were undertaken for the optimized geometries to confirm that they correspond to stationary points featuring no imaginary frequencies. Gibbs free energies were calculated by single point calculations with BP86/def2-TZVP^[7] method on the BP86/def2-SVP geometries.

(S9) Discussion on D→→I Conversion: Key Conformational Changes in Ti–O_aCH(CH₃)O_bCH₃ Fragment :

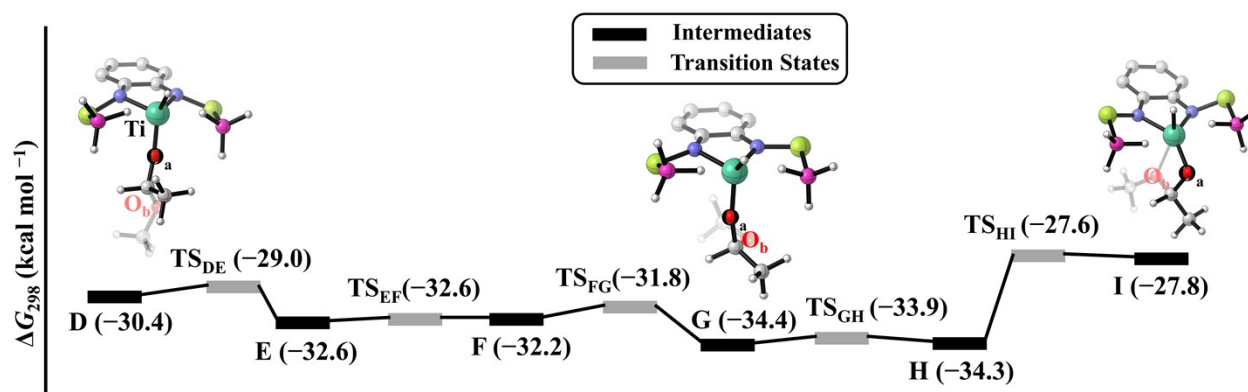
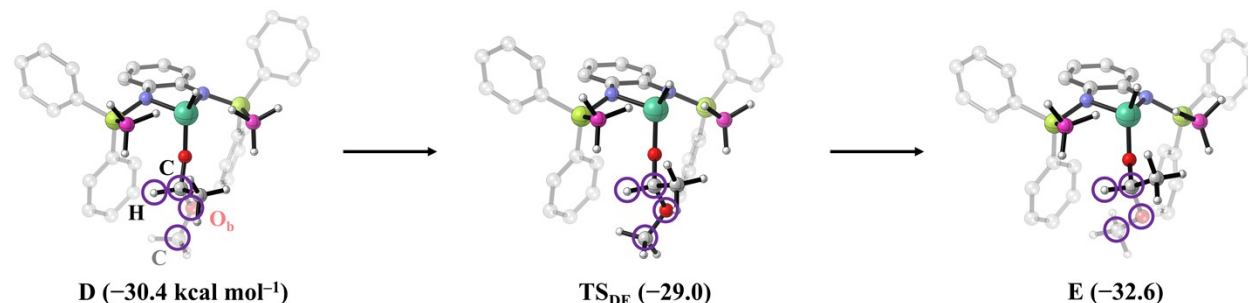


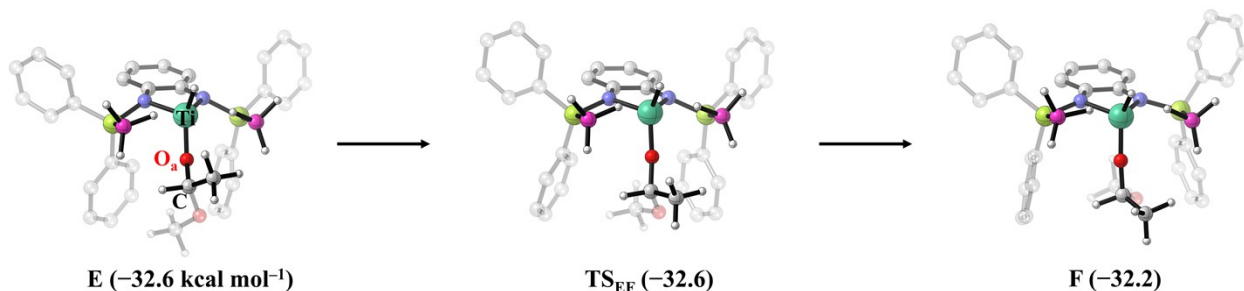
Figure S85. D→→I conversion. Conformational changes occur in the Ti-coordinated CH₃C(O_a)(O_b)CH₃ unit. BP86-D3/def2-TZVP // BP86-D3/def2-SVP is used. Gibbs free energies ΔG₂₉₈ [kcal mol⁻¹] are relative to A.

S9.1. D→TS_{DE}→E: Rotation Around C–O_b Bond



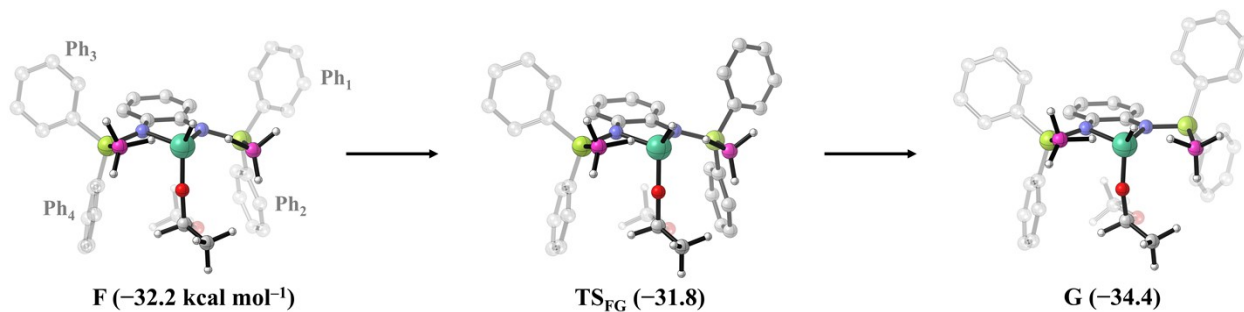
The intermediate **D** is connected to the transition state **TS_{DE}** involving rotation along C–O_b with a minute activation barrier of 1.4 kcal mol⁻¹ to give intermediate **E**. The dihedral angle H–C–O_b–C is –40.44° in **D**, –12.21° in **TS_{DE}** and 45.05° in **E**, respectively which clearly indicate the rotation around –O_bCH₃ fragment.

S9.2. E→TS_{EF}→F: Change in Ti–O_a–C Angle



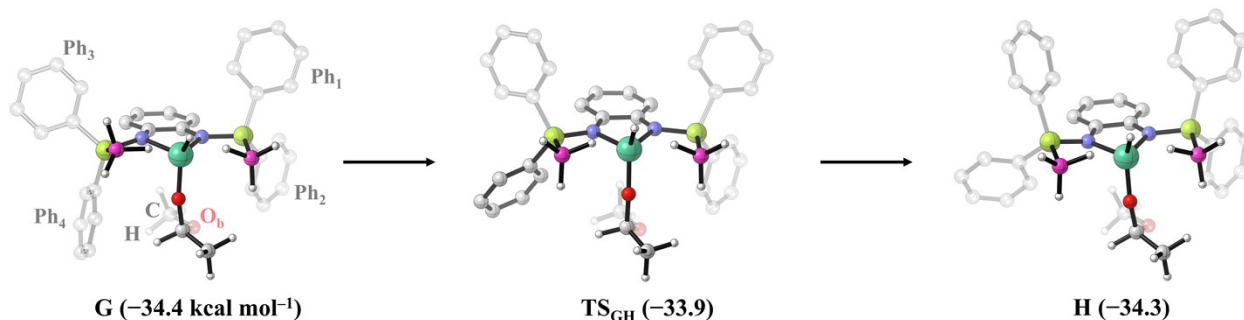
Intermediate **E** undergoes an inward rotation in CH₃CH(O_a)(O_b)CH₃ fragment through **TS_{EF}** with a minute activation barrier of 0.1 kcal mol⁻¹ to produce **F**. This rotation is evidenced by the change in angle of Ti–O_a–C which is 142.37° in **E**, 168.75° in **TS_{EF}** and 199.98° in **F**, respectively.

S9.3. F→TS_{FG}→G: Rotation in Phenyl Rings



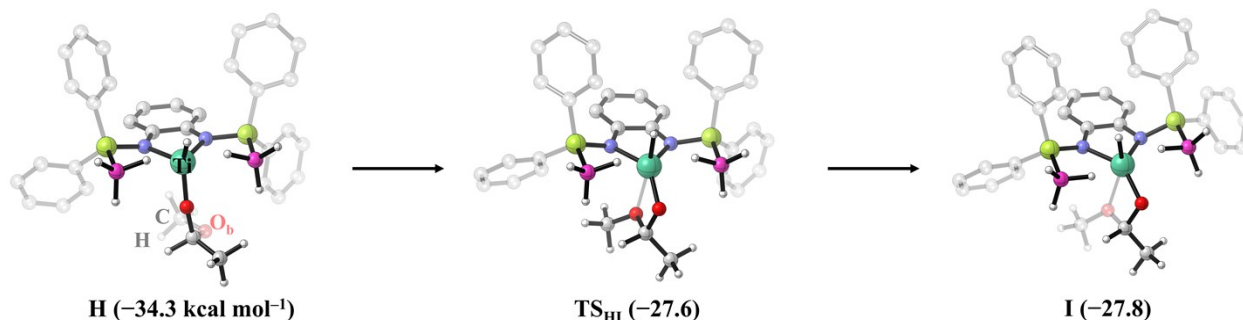
Intermediate **F** is connected to **G** via transition state **TS_{FG}** in which a slight rotation in phenyl rings Ph₁ and Ph₂ takes place leading to an activation barrier of merely 0.44 kcal mol⁻¹. Due to this rotation, these phenyl rings are now oriented in such a way that there is less steric hindrance.

S9.4. G→TS_{GH}→H: Rotation in Phenyl Ring



Intermediate **G** undergoes rotation in phenyl ring Ph₄ via TS_{GH} with an activation barrier of only 0.5 kcal mol⁻¹ to produce **H**. Now, the orientation of all phenyl rings allows the free rotation of (O_b)CH₃ group in the next intermediates and transition states.

S9.5. H→TS_{HI}→I: Rotation of (O_b)CH₃ Group



Now, due to rotation of (O_b)CH₃ group in intermediate **H** via TS_{HI}, coordination of methoxy oxygen (O_b) takes place and leads to the formation of a less stable intermediate **I** (in comparison with **H**). The activation barrier for this conversion is 6.7 kcal mol⁻¹. The Ti–O_b distance is 3.53 Å in **H**, 2.41 Å in TS_{HI} and 2.23 Å in **I** are in line with observation of coordination of O_b to Ti centre.

(S10) Discussion on J→→O Conversion: Key Changes in Acetaldehyde Orientation Around the Ti Center :

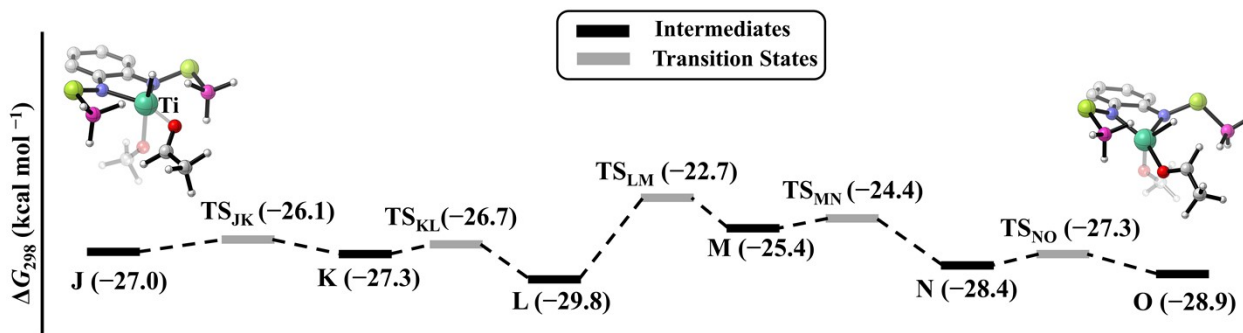
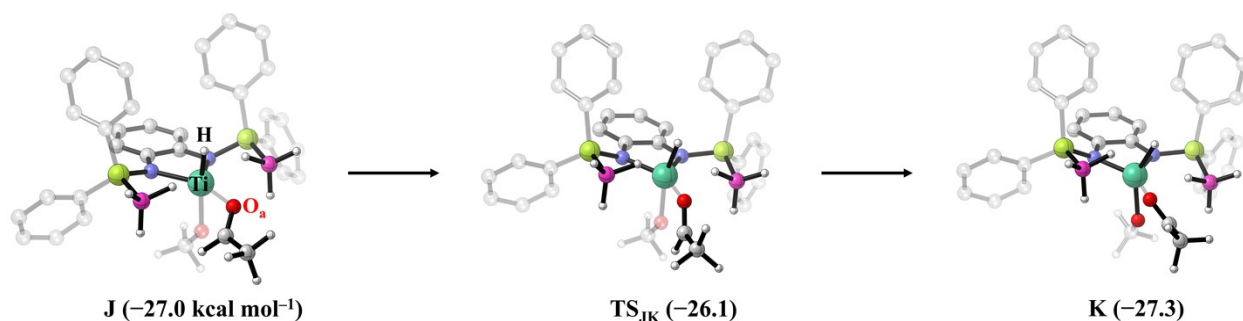


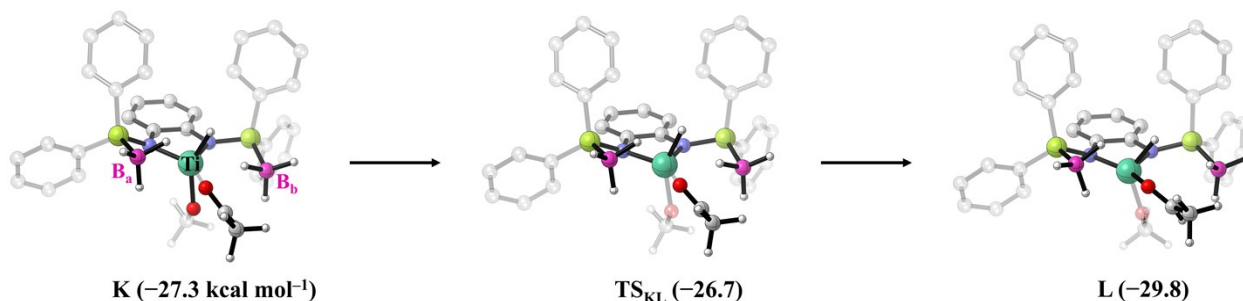
Figure S8. J→→O conversion. Changes in acetaldehyde orientation around the Ti center. BP86-D3/def2-TZVP // BP86-D3/def2-SVP is used. Gibbs free energies ΔG₂₉₈ [kcal mol⁻¹] are relative to **A**.

S10.1. J→TS_{JK}→K: Rotation Around Ti–O_a Bond



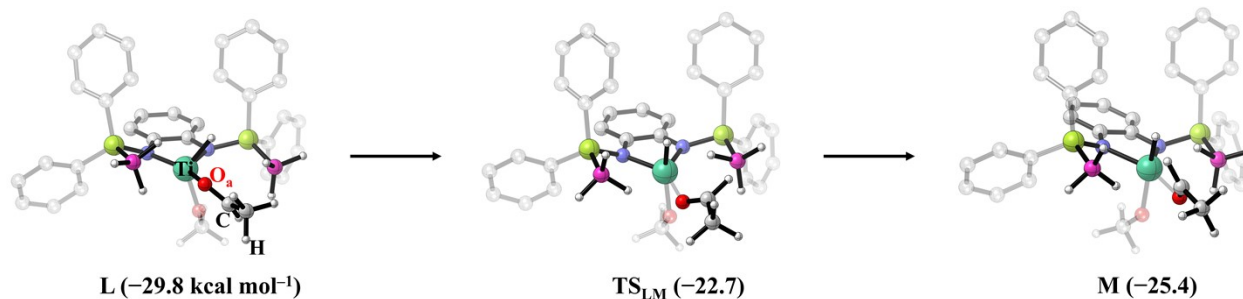
The second intramolecular hydride transfer to carbonyl carbon does not take place until hydride and carbonyl carbon are on the same plane. In intermediate **J**, hydride and carbonyl carbon are in opposite planes. That is the reason, in intermediate **J**, the rotation of $\text{CH}_3\text{C}(\text{O}_a)\text{H}$ fragment around $\text{Ti}-\text{O}_a$ bond occurs via **TS_{JK}** with the activation barrier of only $0.9 \text{ kcal mol}^{-1}$ and leads to intermediate **K**. However, this rotational step is not enough to make them in the same plane.

S10.2. **K**→**TS_{KL}**→**L**: Change in Nonbonding $\text{Ti}-\text{B}_a$ Distance



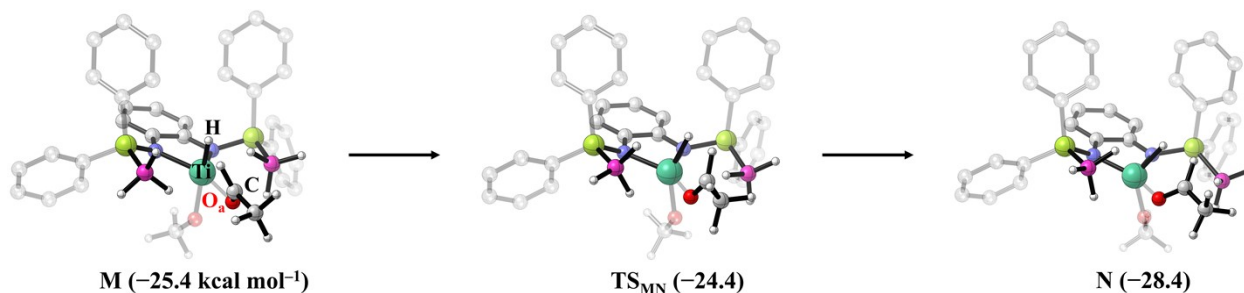
Intermediate **K** is connected to **L** via **TS_{KL}** with the activation barrier of only $0.6 \text{ kcal mol}^{-1}$. The structure of **TS_{KL}** shows a small increase in nonbonding $\text{Ti}-\text{B}_a$ distance from 3.08 \AA upto 3.09 \AA , whereas this distance of 3.57 \AA is found in **L**. The increase in this distance will allow further rotation of $\text{CH}_3\text{C}(\text{O}_a)\text{H}$ fragment around $\text{Ti}-\text{O}_a$ bond.

S10.3. **L**→**TS_{LM}**→**M**: Rotation Around $\text{Ti}-\text{O}_a$ Bond



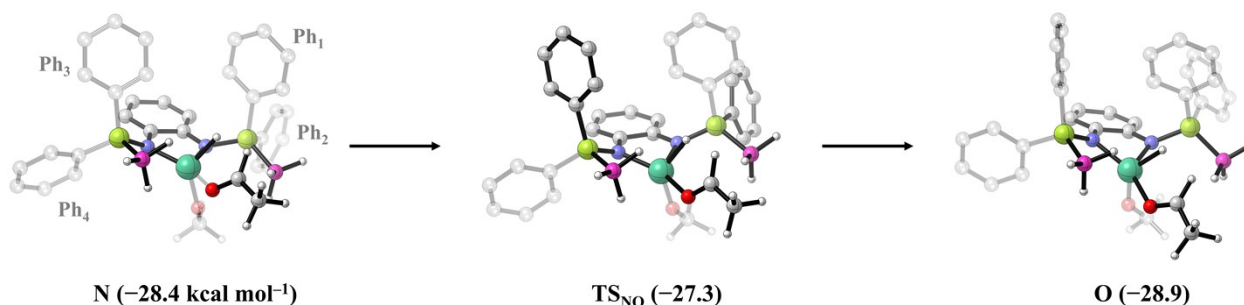
In intermediate **L**, rotation of $\text{CH}_3\text{C}(\text{O}_a)\text{H}$ fragment around $\text{Ti}-\text{O}_a$ bond occurs via **TS_{LM}** to produce **M** with an activation barrier of $7.1 \text{ kcal mol}^{-1}$.

S10.4. M→TS_{MN}→N: Change in dihedral Angle in H–Ti–(O)_a–CHCH₃



Intermediate **M** is connected to **N** via a transition state **TS_{MN}** with an activation barrier of 1 kcal mol^{–1}. The transition state involves the change in dihedral angle in H–Ti–(O)_a–CHCH₃ around Ti–O_a bond. Now, hydride and carbonyl carbon are in one plane for hydride transfer.

S10.5. N→TS_{NO}→O: Rotation in Phenyl Ring



Before hydride transfer to the carbonyl carbon, there is a rotation in Ph₃ (phenyl ring) in **N** connected to **O** via **TS_{NO}** with an activation barrier of 1.1 kcal mol^{–1}. Now, in the subsequent step, there will be a second intramolecular hydride transfer.

(S11) Energy Table for Figure 3:

Total electronic energies and Gibbs free energies (298 K) of the molecules present in Figure 3. Employed DFT method: BP86-D3/def2-TZVP // BP86-D3/def2-SVP.

Molecule	E _{tot} [au]	G ₂₉₈ [au]	Imaginary Frequency
A	–2854.787918	–2854.326820	
B	–268.504041	–268.446473	
C	–3123.309843	–3122.766509	
TS_{CD}	–3123.306837	–3122.762590	<i>i</i> 40
D	–3123.369182	–3122.821740	
G	–3123.377585	–3122.828109	

I	-3123.367052	-3122.817575	
TS_{IJ}	-3123.348813	-3122.803809	<i>i95</i>
J	-3123.358379	-3122.816335	
O	-3123.361247	-3122.819353	
TS_{OP}	-3123.356828	-3122.813810	<i>i104</i>
P	-3123.443789	-3122.895992	

(S12) Energy Table for Figure S85:

Total electronic energies and Gibbs free energies (298 K) of the molecules present in Figure S85. Employed DFT method: BP86-D3/def2-TZVP // BP86-D3/def2-SVP.

Molecule	E_{tot} [au]	G_{298} [au]	Imaginary Frequency
D	-3123.369182	-3122.821740	
TS_{DE}	-3123.368894	-2854.819547	<i>i50</i>
E	-3123.373775	-3122.825288	
TS_{EF}	-3123.373872	-3122.825185	<i>i22</i>
F	-3123.374158	-3122.824671	
TS_{FG}	-3123.373954	-3122.823910	<i>i20</i>
G	-3123.377585	-3122.828109	
TS_{GH}	-3123.375910	-3122.827240	<i>i13</i>
H	-3123.375541	-3122.827936	
TS_{HI}	-3123.356828	-3122.817276	<i>i35</i>
I	-3123.367052	-3122.817575	

(S13) Energy Table for Figure S86:

Total electronic energies and Gibbs free energies (298 K) of the molecules present in Figure S86. Employed DFT method: BP86-D3/def2-TZVP // BP86-D3/def2-SVP.

Molecule	E_{tot} [au]	G_{298} [au]	Imaginary Frequency
J	-3123.358379	-3122.816335	
TS_{JK}	-3123.356931	-2854.814808	<i>i54</i>

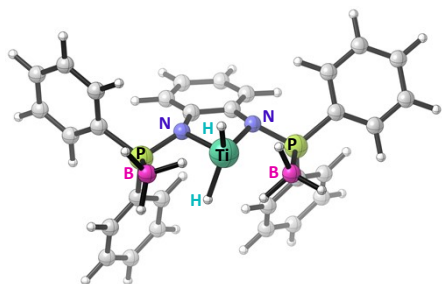
K	-3123.359765	-3122.816802	
TS_{KL}	-3123.359810	-3122.815886	<i>i27</i>
L	-3123.364657	-3122.820833	
TS_{LM}	-3123.352110	-3122.809519	<i>i59</i>
M	-3123.355120	-3122.813712	
TS_{MN}	-3123.353605	-3122.812123	<i>i99</i>
N	-3123.360687	-3122.818571	
TS_{NO}	-3123.360000	-3122.816860	<i>i14</i>
O	-3123.361247	-3122.819353	

(S14) Cartesian Coordinates of the Optimized Structures

DFT optimization method: BP86-D3/def2-SVP

S14.1 XYZ coordinates of the molecules present in Figure 3

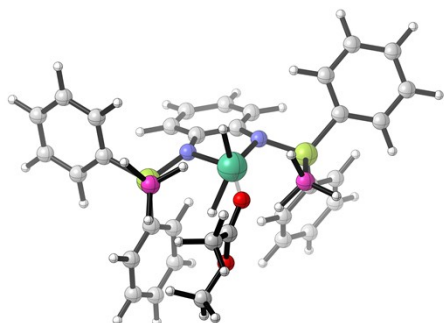
A



Ti	7.491971000	1.325268000	30.089011000
H	8.513558000	0.691927000	28.869795000
H	7.790000000	1.634897000	31.751005000
P	8.713972000	3.945357000	30.675057000
P	4.758704000	0.403634000	30.068667000
N	7.414631000	3.318732000	29.797418000
N	5.581338000	1.712937000	29.444898000
C	6.220438000	3.960610000	29.444852000
C	5.148405000	3.031486000	29.279880000
C	3.847159000	3.490314000	29.009564000
H	3.016561000	2.774046000	28.921254000
C	3.619323000	4.871504000	28.864857000
H	2.602913000	5.234279000	28.650004000
C	4.681154000	5.784698000	28.989944000
H	4.495614000	6.862755000	28.867968000
C	5.983402000	5.339058000	29.281597000
H	6.804906000	6.057083000	29.402805000
C	9.286929000	5.467458000	29.824071000
C	9.699667000	5.326838000	28.481716000
H	9.688665000	4.331992000	28.009699000
C	10.106248000	6.453093000	27.752931000
H	10.421550000	6.340530000	26.704747000
C	10.113764000	7.721678000	28.360370000
H	10.436060000	8.604444000	27.787517000
C	9.710119000	7.861766000	29.698201000

H	9.714536000	8.853842000	30.175619000
C	9.292771000	6.738445000	30.431511000
H	8.959256000	6.852382000	31.473334000
C	8.122630000	4.504896000	32.312109000
C	9.079744000	4.826162000	33.297007000
H	10.153422000	4.731169000	33.070808000
C	8.663195000	5.250081000	34.568969000
H	9.412944000	5.496996000	35.335993000
C	7.292569000	5.349076000	34.863740000
H	6.966369000	5.683447000	35.860382000
C	6.339453000	5.014901000	33.886469000
H	5.264309000	5.088560000	34.112190000
C	6.748650000	4.589124000	32.612936000
H	5.999305000	4.321610000	31.854773000
C	3.625424000	-0.339740000	28.855371000
C	2.932366000	-1.526421000	29.175873000
H	3.058646000	-1.992995000	30.165897000
C	2.090166000	-2.118166000	28.222789000
H	1.550910000	-3.044966000	28.469761000
C	1.947310000	-1.535426000	26.950814000
H	1.288723000	-2.003648000	26.203434000
C	2.653982000	-0.365178000	26.627046000
H	2.551475000	0.084039000	25.627759000
C	3.499412000	0.233510000	27.574677000
H	4.070164000	1.140501000	27.326551000
C	3.771214000	0.988697000	31.490643000
C	2.366568000	0.904342000	31.543577000
H	1.810500000	0.424090000	30.724224000
C	1.677046000	1.443861000	32.642555000
H	0.578846000	1.377024000	32.683267000
C	2.384726000	2.070730000	33.681132000
H	1.841551000	2.492076000	34.540968000
C	3.787123000	2.164552000	33.621571000
H	4.347956000	2.657850000	34.429791000
C	4.483290000	1.628401000	32.529885000
H	5.582671000	1.720307000	32.478826000
B	10.013977000	2.515650000	30.695984000
H	9.449492000	1.504337000	30.176384000
H	10.410119000	2.334074000	31.835625000
H	10.868523000	2.793376000	29.862202000
B	6.283798000	-0.688907000	30.534436000
H	6.857416000	-0.042460000	31.450244000
H	7.007340000	-0.629320000	29.509535000
H	6.026990000	-1.822703000	30.884540000

C

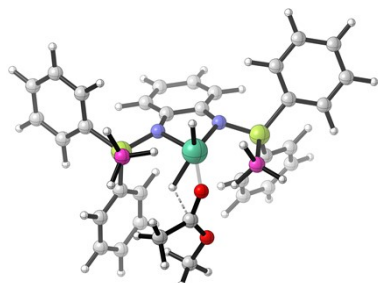


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P	4.883809000	0.174107000	29.959932000
N	7.410973000	3.149985000	31.044886000
N	5.558656000	1.569124000	30.617614000

C	6.241211000	3.805010000	30.649350000
C	5.170147000	2.892036000	30.408590000
C	3.921205000	3.391142000	29.976183000
H	3.089684000	2.703481000	29.778308000
C	3.754088000	4.772988000	29.778080000
H	2.779396000	5.151976000	29.434485000
C	4.816136000	5.667060000	30.003242000
H	4.677864000	6.745892000	29.834177000
C	6.063609000	5.184865000	30.437820000
H	6.901963000	5.877583000	30.601544000
C	8.979636000	4.352947000	29.034548000
C	8.514584000	3.479076000	28.025700000
H	8.192184000	2.456731000	28.283091000
C	8.439620000	3.922476000	26.698738000
H	8.079227000	3.234914000	25.919156000
C	8.818871000	5.236124000	26.368839000
H	8.754912000	5.582707000	25.325924000
C	9.269293000	6.108783000	27.372458000
H	9.555398000	7.140944000	27.119543000
C	9.347222000	5.671400000	28.705596000
H	9.683071000	6.364206000	29.491580000
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C	10.747882000	5.594238000	31.795898000
H	11.461739000	5.244122000	31.033288000
C	11.126589000	6.595857000	32.702736000
H	12.133033000	7.037046000	32.642733000
C	10.224090000	7.028842000	33.690593000
H	10.522605000	7.815622000	34.400509000
C	8.946029000	6.451683000	33.779799000
H	8.243390000	6.780785000	34.560476000
C	8.559348000	5.450172000	32.875348000
H	7.567120000	4.979564000	32.941895000
C	5.151683000	0.160424000	28.147226000
C	5.130266000	-1.070821000	27.462333000
H	4.951278000	-2.001985000	28.021795000
C	5.352393000	-1.108112000	26.075680000
H	5.335841000	-2.072212000	25.543420000
C	5.596840000	0.081996000	25.369087000
H	5.773173000	0.051826000	24.282658000
C	5.615277000	1.310710000	26.052972000
H	5.799656000	2.246873000	25.503944000
C	5.395334000	1.354771000	27.437984000
H	5.419836000	2.315763000	27.972996000
C	3.058132000	0.256999000	30.153744000
C	2.160254000	0.156808000	29.072865000
H	2.544634000	0.028122000	28.050210000
C	0.775854000	0.238088000	29.299996000
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H	-0.799930000	0.498550000	30.777969000
C	1.180066000	0.524268000	31.683139000
H	0.797458000	0.675370000	32.704171000
C	2.561051000	0.434238000	31.463299000
H	3.266220000	0.517802000	32.304881000
B	9.818742000	1.989638000	30.975054000
H	9.339975000	1.636444000	32.074559000
H	11.030855000	1.918168000	30.928732000
H	9.281786000	1.319482000	30.060449000
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H	6.514828000	-0.617587000	31.690060000
H	6.176195000	-2.100604000	30.232302000
H	4.863630000	-1.663525000	31.774109000
O	8.826873000	-0.736911000	31.396595000
C	8.941676000	-1.735531000	30.687447000
H	7.333200000	0.261829000	29.631718000
O	8.917809000	-1.595131000	29.357680000
C	8.748737000	-2.718942000	28.490974000

H	9.612994000	-3.414034000	28.539713000
H	7.809855000	-3.258798000	28.730386000
H	8.669720000	-2.300553000	27.471953000
C	9.093133000	-3.109390000	31.284391000
H	8.127055000	-3.643653000	31.164096000
H	9.883874000	-3.707884000	30.791217000
H	9.302535000	-3.003779000	32.362167000

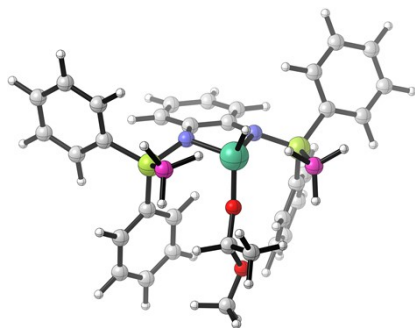
TS_{CD}



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P	4.813453000	0.082636000	30.223865000
N	7.430372000	3.097720000	30.994653000
N	5.574714000	1.520877000	30.657861000
C	6.275473000	3.743488000	30.549654000
C	5.200660000	2.826685000	30.345291000
C	3.967652000	3.307945000	29.850963000
H	3.133866000	2.617554000	29.673902000
C	3.816519000	4.677492000	29.570905000
H	2.853588000	5.042412000	29.182058000
C	4.879023000	5.576298000	29.772973000
H	4.753241000	6.644713000	29.540901000
C	6.113133000	5.111306000	30.260548000
H	6.953233000	5.806420000	30.402352000
C	9.091164000	4.338031000	29.085145000
C	8.602153000	3.499147000	28.058495000
H	8.208179000	2.500155000	28.305977000
C	8.595646000	3.948418000	26.731728000
H	8.209357000	3.291888000	25.937506000
C	9.073498000	5.233659000	26.418710000
H	9.063594000	5.586729000	25.376069000
C	9.553381000	6.070601000	27.438969000
H	9.916988000	7.080977000	27.198204000
C	9.559847000	5.627448000	28.772553000
H	9.916071000	6.294954000	29.571168000
C	9.396783000	5.008776000	31.944941000
C	10.703137000	5.542909000	31.980376000
H	11.477228000	5.162142000	31.295269000
C	11.018508000	6.553730000	32.901204000
H	12.035701000	6.973145000	32.926655000
C	10.039141000	7.021989000	33.795074000
H	10.288595000	7.815626000	34.516135000
C	8.746915000	6.470062000	33.777626000
H	7.983723000	6.825617000	34.486426000
C	8.422801000	5.459938000	32.858188000
H	7.419178000	5.009712000	32.845764000
C	5.108550000	-0.220084000	28.437340000
C	5.043088000	-1.537012000	27.941944000
H	4.771708000	-2.360231000	28.620463000
C	5.348888000	-1.798051000	26.595090000
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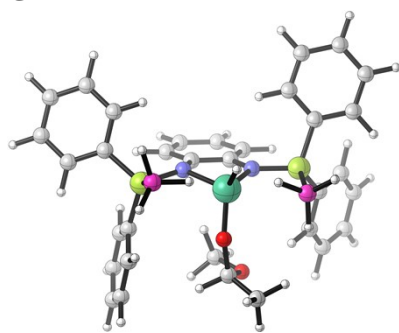
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C	5.465974000	0.837584000	27.575517000
H	5.528267000	1.864908000	27.965100000
C	2.993812000	0.270627000	30.365405000
C	2.117014000	0.076905000	29.279279000
H	2.519003000	-0.197397000	28.292632000
C	0.733996000	0.250517000	29.453770000
H	0.053165000	0.097671000	28.602264000
C	0.223411000	0.625754000	30.707451000
H	-0.859884000	0.771692000	30.840193000
C	1.097049000	0.817642000	31.793343000
H	0.699163000	1.115010000	32.775555000
C	2.476557000	0.633966000	31.627897000
H	3.164337000	0.787075000	32.473387000
B	9.828950000	1.960784000	31.039328000
H	9.297282000	1.585981000	32.110925000
H	11.038685000	1.863237000	31.039165000
H	9.309588000	1.332177000	30.089720000
B	5.544539000	-1.185981000	31.454625000
H	6.584923000	-0.615940000	31.892117000
H	5.757463000	-2.261981000	30.915934000
H	4.779291000	-1.220408000	32.410579000
O	8.925094000	-0.825721000	31.338313000
C	8.953055000	-1.495034000	30.302491000
H	7.256098000	0.065164000	29.738474000
O	9.518237000	-0.967151000	29.200108000
C	9.167501000	-1.463891000	27.902891000
H	9.456124000	-2.527014000	27.768768000
H	8.077733000	-1.338782000	27.730191000
H	9.726209000	-0.843557000	27.180846000
C	8.438377000	-2.906707000	30.237194000
H	7.474639000	-2.897948000	29.689360000
H	9.140398000	-3.583572000	29.711424000
H	8.240865000	-3.260615000	31.262145000

D



Ti	7.231252000	0.994663000	31.425273000
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P	8.960734000	3.443226000	31.003195000
P	4.590441000	0.172473000	30.335695000
N	7.339857000	3.015705000	31.204363000
N	5.335310000	1.559246000	30.930647000
C	6.227506000	3.723869000	30.717663000
C	5.081736000	2.890880000	30.555114000
C	3.882307000	3.434945000	30.062995000
H	3.000721000	2.794899000	29.931693000
C	3.823652000	4.802518000	29.732335000
H	2.884504000	5.222517000	29.341560000
C	4.949224000	5.624642000	29.896947000
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C	6.153981000	5.089907000	30.392746000

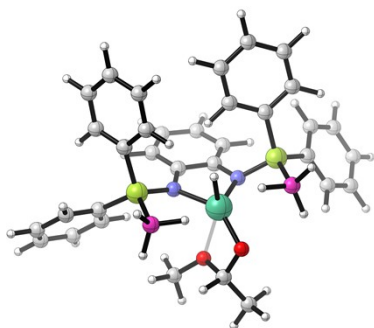
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H	9.253256000	1.718898000	28.705983000
C	9.273528000	2.990077000	26.956753000
H	9.321665000	2.131645000	26.270029000
C	9.253475000	4.304275000	26.457467000
H	9.280626000	4.484868000	25.371387000
C	9.201048000	5.390132000	27.347110000
H	9.180957000	6.420863000	26.961429000
C	9.165020000	5.164807000	28.732359000
H	9.117241000	6.019535000	29.423404000
C	9.304164000	4.967040000	31.948671000
C	10.508128000	5.674742000	31.749392000
H	11.225288000	5.343702000	30.981909000
C	10.790629000	6.804322000	32.532159000
H	11.727776000	7.359392000	32.373547000
C	9.880671000	7.224337000	33.518522000
H	10.102317000	8.113394000	34.128388000
C	8.690538000	6.507678000	33.729149000
H	7.979737000	6.829948000	34.505323000
C	8.401535000	5.376793000	32.949649000
H	7.474200000	4.805054000	33.106262000
C	4.940232000	0.061958000	28.542320000
C	4.499157000	-1.064810000	27.814916000
H	3.906505000	-1.847915000	28.314267000
C	4.820875000	-1.191508000	26.454935000
H	4.471716000	-2.069422000	25.890032000
C	5.597584000	-0.204422000	25.821095000
H	5.855668000	-0.308336000	24.756020000
C	6.054681000	0.904993000	26.550652000
H	6.677941000	1.673417000	26.069576000
C	5.729974000	1.041504000	27.908248000
H	6.104053000	1.904771000	28.475075000
C	2.770044000	0.312393000	30.491509000
C	1.906805000	0.426118000	29.383043000
H	2.314888000	0.393353000	28.362104000
C	0.528480000	0.601993000	29.585623000
H	-0.142876000	0.691866000	28.718106000
C	0.010599000	0.674159000	30.889660000
H	-1.069185000	0.821628000	31.046331000
C	0.871338000	0.561153000	31.995647000
H	0.467305000	0.618514000	33.017829000
C	2.246944000	0.374327000	31.800355000
H	2.924289000	0.285582000	32.663548000
B	9.883014000	1.874912000	31.657034000
H	8.985259000	1.246604000	32.299870000
H	10.651883000	2.228314000	32.539450000
H	10.380465000	1.246954000	30.740011000
B	5.398115000	-1.210679000	31.413364000
H	6.316794000	-0.630704000	32.069377000
H	5.818193000	-2.123664000	30.720036000
H	4.592364000	-1.529563000	32.277877000
O	7.860114000	0.063564000	30.041682000
C	8.250115000	-1.008979000	29.251604000
H	7.328419000	-1.569577000	28.948662000
O	8.847673000	-0.451777000	28.085529000
C	8.830349000	-1.311279000	26.965645000
H	9.475116000	-2.211145000	27.103657000
H	7.795933000	-1.651019000	26.725055000
H	9.220786000	-0.736489000	26.103695000
C	9.211945000	-1.909075000	30.020850000
H	8.704926000	-2.324315000	30.912895000
H	9.557435000	-2.753518000	29.391104000
H	10.085858000	-1.312606000	30.345644000

G

Ti	0.288927000	-1.517522000	1.333591000
H	0.430224000	-2.031953000	2.954796000
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P	-2.671014000	-1.098440000	0.688407000
N	1.247324000	0.155591000	0.675610000
N	-1.213223000	-0.255439000	0.685964000
C	0.539165000	1.138799000	-0.031123000
C	-0.868455000	0.894463000	-0.039951000
C	-1.723941000	1.796060000	-0.702864000
H	-2.810368000	1.636019000	-0.685415000
C	-1.189025000	2.921702000	-1.357443000
H	-1.866492000	3.620365000	-1.871326000
C	0.194763000	3.157794000	-1.347425000
H	0.611040000	4.040336000	-1.856086000
C	1.061747000	2.270875000	-0.682534000
H	2.143717000	2.459047000	-0.676068000
C	3.854385000	0.478287000	-0.508063000
C	3.689006000	-0.421109000	-1.583387000
H	3.021369000	-1.293271000	-1.484067000
C	4.360789000	-0.185515000	-2.792255000
H	4.225356000	-0.885558000	-3.631392000
C	5.201635000	0.932521000	-2.932531000
H	5.727461000	1.111383000	-3.882969000
C	5.369284000	1.823204000	-1.858969000
H	6.024143000	2.701826000	-1.965498000
C	4.694991000	1.601037000	-0.647234000
H	4.815174000	2.308049000	0.187624000
C	3.282962000	1.460975000	2.188977000
C	4.582511000	1.544920000	2.733567000
H	5.356118000	0.822624000	2.428078000
C	4.883829000	2.539783000	3.675845000
H	5.897411000	2.602363000	4.100073000
C	3.888612000	3.444098000	4.087492000
H	4.125477000	4.220525000	4.831282000
C	2.589943000	3.348260000	3.560258000
H	1.806088000	4.046760000	3.890459000
C	2.282533000	2.357150000	2.613945000
H	1.264846000	2.273187000	2.206295000
C	-2.933778000	-1.865061000	-0.954016000
C	-2.850379000	-3.268968000	-1.061636000
H	-2.695526000	-3.867784000	-0.151740000
C	-2.960109000	-3.887919000	-2.317528000
H	-2.897741000	-4.984703000	-2.393097000
C	-3.149726000	-3.111250000	-3.472507000
H	-3.236355000	-3.597661000	-4.456245000
C	-3.231276000	-1.711214000	-3.370699000
H	-3.378489000	-1.099391000	-4.273597000
C	-3.126653000	-1.087444000	-2.118562000
H	-3.187480000	0.007506000	-2.049152000
C	-4.054908000	0.073535000	0.921546000
C	-5.285191000	-0.066412000	0.249753000
H	-5.426867000	-0.878716000	-0.479607000

C	-6.331109000	0.834741000	0.511354000
H	-7.291939000	0.723393000	-0.013876000
C	-6.150960000	1.873597000	1.439046000
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C	-4.924576000	2.009037000	2.115074000
H	-4.782494000	2.822344000	2.843279000
C	-3.879918000	1.109243000	1.864095000
H	-2.915503000	1.209814000	2.385539000
B	3.095659000	-1.659672000	1.697938000
H	1.986007000	-1.839434000	2.299309000
H	3.919412000	-1.706419000	2.599683000
H	3.290310000	-2.412707000	0.759295000
B	-2.402888000	-2.310233000	2.152728000
H	-1.155412000	-2.313537000	2.386284000
H	-2.790924000	-3.446926000	1.934873000
H	-2.894151000	-1.761732000	3.129288000
O	0.361007000	-2.887663000	0.203499000
C	0.706012000	-3.462487000	-1.042615000
H	-0.249478000	-3.836354000	-1.486416000
C	1.706260000	-4.585370000	-0.830500000
H	1.283627000	-5.342005000	-0.142892000
H	1.951760000	-5.062237000	-1.798769000
H	2.628334000	-4.171233000	-0.380659000
O	1.277873000	-2.512076000	-1.904899000
C	0.361014000	-1.537109000	-2.389579000
H	-0.405100000	-1.999104000	-3.052240000
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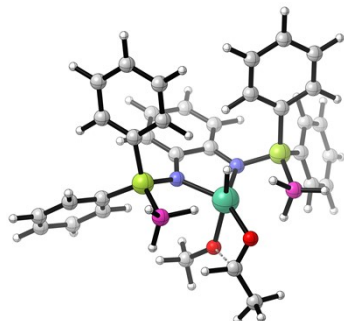
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P	5.009664000	0.033316000	29.816179000
N	8.084340000	2.748352000	29.509462000
N	6.111848000	1.189894000	29.306137000
C	6.981762000	3.323698000	28.845902000
C	5.844664000	2.461937000	28.792161000
C	4.624631000	2.952110000	28.284888000
H	3.729500000	2.316064000	28.292864000
C	4.549704000	4.263918000	27.782314000
H	3.592413000	4.637142000	27.388273000
C	5.685497000	5.089498000	27.780353000
H	5.629590000	6.108355000	27.369206000
C	6.900459000	4.623519000	28.315915000
H	7.784697000	5.273045000	28.324843000
C	10.070531000	4.905043000	29.681843000
C	11.250756000	4.490725000	29.029107000
H	11.564572000	3.438210000	29.097560000
C	12.020797000	5.417506000	28.309631000
H	12.942245000	5.087269000	27.806656000
C	11.622757000	6.763247000	28.242072000

H	12.230553000	7.490520000	27.682242000
C	10.450698000	7.181934000	28.895619000
H	10.137003000	8.236003000	28.846111000
C	9.674759000	6.258318000	29.611909000
H	8.755004000	6.588723000	30.116741000
C	8.012226000	4.496947000	31.732925000
C	8.536088000	5.507426000	32.567062000
H	9.586735000	5.819111000	32.465172000
C	7.719117000	6.113796000	33.533847000
H	8.133583000	6.902130000	34.181053000
C	6.379169000	5.713551000	33.676119000
H	5.738245000	6.195705000	34.430443000
C	5.862881000	4.692490000	32.861333000
H	4.819868000	4.361500000	32.970296000
C	6.676152000	4.077723000	31.898026000
H	6.272786000	3.261185000	31.283294000
C	3.900600000	-0.537641000	28.475524000
C	2.946538000	-1.531953000	28.783573000
H	2.844158000	-1.893507000	29.818947000
C	2.135054000	-2.065361000	27.771273000
H	1.393560000	-2.841053000	28.017347000
C	2.274431000	-1.616383000	26.445867000
H	1.638370000	-2.036894000	25.652238000
C	3.229415000	-0.634256000	26.135182000
H	3.341604000	-0.280093000	25.099064000
C	4.044101000	-0.097317000	27.145320000
H	4.788061000	0.674845000	26.903373000
C	3.912772000	0.842205000	31.042936000
C	2.602343000	1.260549000	30.736472000
H	2.172421000	1.039016000	29.748366000
C	1.843051000	1.951135000	31.695111000
H	0.821144000	2.277515000	31.450391000
C	2.387447000	2.223199000	32.961054000
H	1.788877000	2.759032000	33.713878000
C	3.695212000	1.806142000	33.268910000
H	4.123741000	2.014331000	34.260863000
C	4.460169000	1.119394000	32.314898000
H	5.491463000	0.808458000	32.545445000
B	10.127243000	2.226520000	31.367249000
H	9.196893000	1.404247000	31.611668000
H	10.526757000	2.590951000	32.462916000
H	10.962905000	1.815564000	30.579955000
B	6.099107000	-1.403491000	30.495413000
H	7.158946000	-0.857051000	30.879077000
H	6.288059000	-2.203943000	29.591224000
H	5.575051000	-1.868167000	31.497737000
O	9.453110000	-0.415063000	30.031503000
C	9.270021000	-1.153299000	28.890097000
H	8.824588000	-2.159349000	29.101198000
C	10.529543000	-1.256511000	28.045534000
H	11.309106000	-1.789859000	28.623464000
H	10.349546000	-1.816717000	27.105932000
H	10.893768000	-0.238520000	27.807414000
O	8.239992000	-0.355808000	28.207303000
C	7.464958000	-0.968413000	27.186371000
H	8.125301000	-1.353350000	26.380612000
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H	6.809221000	-0.185380000	26.767906000

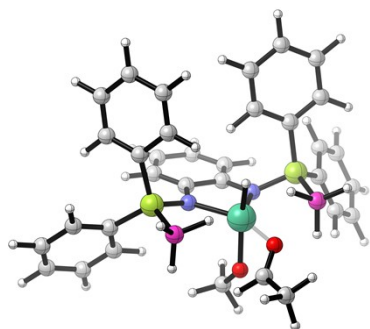
TS_{IJ}



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P	4.959470000	-0.006935000	29.674197000
N	7.884128000	2.880938000	29.552338000
N	6.067525000	1.206975000	29.269324000
C	6.732115000	3.442384000	28.995849000
C	5.681022000	2.489180000	28.862321000
C	4.418680000	2.911373000	28.395206000
H	3.589428000	2.197381000	28.311556000
C	4.217502000	4.255626000	28.038445000
H	3.230071000	4.574322000	27.671932000
C	5.264108000	5.187043000	28.148291000
H	5.103678000	6.236901000	27.860285000
C	6.521268000	4.785460000	28.631506000
H	7.336617000	5.513596000	28.725791000
C	9.916406000	4.992055000	29.423555000
C	10.924874000	4.546301000	28.542814000
H	11.184239000	3.476700000	28.511060000
C	11.593211000	5.463530000	27.718101000
H	12.379545000	5.110309000	27.033355000
C	11.265707000	6.829219000	27.772358000
H	11.794335000	7.547925000	27.127622000
C	10.265974000	7.277907000	28.652676000
H	10.007159000	8.347043000	28.696883000
C	9.590647000	6.364119000	29.475436000
H	8.804735000	6.717805000	30.159773000
C	8.232424000	4.573352000	31.800276000
C	8.922187000	5.516025000	32.592153000
H	9.955431000	5.800296000	32.341352000
C	8.291571000	6.086979000	33.708828000
H	8.833549000	6.819325000	34.326709000
C	6.975816000	5.719356000	34.040176000
H	6.483486000	6.170394000	34.915127000
C	6.294356000	4.769898000	33.260181000
H	5.266596000	4.471104000	33.514262000
C	6.919675000	4.189641000	32.146876000
H	6.395222000	3.427924000	31.553174000
C	3.943791000	-0.491480000	28.233787000
C	2.915047000	-1.441079000	28.415485000
H	2.690198000	-1.823581000	29.423321000
C	2.186933000	-1.906875000	27.310120000
H	1.383270000	-2.644675000	27.457799000
C	2.489297000	-1.439710000	26.019099000
H	1.918248000	-1.807403000	25.153176000
C	3.526467000	-0.510017000	25.834648000
H	3.770648000	-0.147602000	24.824587000
C	4.255941000	-0.037711000	26.936944000
H	5.071449000	0.686749000	26.796303000
C	3.828551000	0.763886000	30.895425000
C	2.463186000	1.016803000	30.663178000
H	1.999862000	0.715561000	29.712040000
C	1.693263000	1.664037000	31.644164000
H	0.627362000	1.864361000	31.456213000

C	2.282968000	2.061858000	32.855008000
H	1.676566000	2.566123000	33.623302000
C	3.648571000	1.815068000	33.084945000
H	4.114576000	2.121919000	34.034037000
C	4.423209000	1.169160000	32.111072000
H	5.501928000	0.993128000	32.270464000
B	10.054378000	2.150930000	30.901896000
H	9.115064000	1.592111000	31.533363000
H	11.014270000	2.251739000	31.640827000
H	10.268716000	1.614545000	29.812535000
B	6.036367000	-1.442993000	30.331146000
H	6.987232000	-0.801560000	30.831596000
H	6.343540000	-2.136720000	29.370377000
H	5.461503000	-2.025376000	31.240973000
O	9.330246000	-0.648546000	30.736762000
C	9.345723000	-1.559724000	29.871883000
H	8.436090000	-2.184941000	29.706272000
C	10.630071000	-2.039706000	29.270335000
H	10.990890000	-2.910785000	29.861017000
H	10.462223000	-2.391461000	28.233986000
H	11.396253000	-1.242625000	29.299555000
O	8.496724000	-0.186598000	28.475041000
C	7.863971000	-0.422246000	27.249401000
H	8.578293000	-0.890816000	26.531988000
H	6.989426000	-1.105187000	27.360200000
H	7.498768000	0.527678000	26.796381000

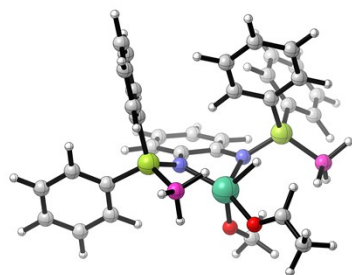
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Ti	7.952068000	0.871299000	29.823458000
H	7.704802000	0.677004000	31.539254000
P	9.053668000	3.713992000	30.220023000
P	4.944118000	-0.017721000	29.610651000
N	7.881564000	2.874107000	29.342907000
N	6.012112000	1.228220000	29.214169000
C	6.712349000	3.432007000	28.806925000
C	5.632143000	2.501604000	28.770536000
C	4.359233000	2.927242000	28.341054000
H	3.514189000	2.227157000	28.334210000
C	4.170443000	4.255397000	27.919474000
H	3.174056000	4.578514000	27.582247000
C	5.243791000	5.160993000	27.923027000
H	5.096642000	6.195784000	27.578877000
C	6.514352000	4.754430000	28.368785000
H	7.350792000	5.464457000	28.372577000
C	9.819462000	5.078652000	29.266673000
C	10.828276000	4.726728000	28.344717000
H	11.136767000	3.673752000	28.254142000
C	11.435212000	5.715509000	27.555664000
H	12.221704000	5.435468000	26.837940000
C	11.046668000	7.059652000	27.687971000
H	11.527292000	7.834967000	27.072086000
C	10.046938000	7.414982000	28.610247000

H	9.741122000	8.467250000	28.715618000
C	9.432028000	6.429376000	29.396765000
H	8.642932000	6.706737000	30.111944000
C	8.200720000	4.478437000	31.645428000
C	8.865584000	5.403018000	32.478494000
H	9.886424000	5.733463000	32.233451000
C	8.227887000	5.895659000	33.627687000
H	8.751232000	6.614325000	34.277088000
C	6.928687000	5.467271000	33.951728000
H	6.430709000	5.857734000	34.852305000
C	6.271827000	4.534998000	33.131276000
H	5.258167000	4.187018000	33.378372000
C	6.905543000	4.033777000	31.984618000
H	6.397130000	3.287536000	31.358166000
C	3.830866000	-0.415448000	28.219663000
C	2.707133000	-1.242299000	28.431834000
H	2.455572000	-1.583798000	29.447869000
C	1.914202000	-1.639508000	27.343745000
H	1.035002000	-2.279524000	27.514425000
C	2.244827000	-1.225603000	26.041930000
H	1.620786000	-1.537346000	25.190663000
C	3.376311000	-0.419947000	25.827484000
H	3.641444000	-0.099367000	24.808613000
C	4.172252000	-0.018036000	26.910824000
H	5.059805000	0.611586000	26.749749000
C	3.922335000	0.663618000	30.971441000
C	2.579713000	1.067227000	30.836598000
H	2.046819000	0.908905000	29.887415000
C	1.920650000	1.681766000	31.914664000
H	0.873200000	2.000183000	31.802890000
C	2.598244000	1.897694000	33.125629000
H	2.079169000	2.379100000	33.968798000
C	3.941368000	1.501563000	33.259323000
H	4.477616000	1.670673000	34.205794000
C	4.605775000	0.888583000	32.187563000
H	5.669935000	0.609731000	32.274527000
B	10.153663000	2.223663000	30.670024000
H	9.220359000	1.551010000	31.201566000
H	10.959690000	2.410813000	31.565336000
H	10.587725000	1.765221000	29.622645000
B	6.135656000	-1.447203000	30.046972000
H	7.031175000	-0.787297000	30.627909000
H	6.475488000	-1.945606000	28.983571000
H	5.662201000	-2.209694000	30.879580000
O	9.416385000	-0.688496000	30.638782000
C	9.507715000	-1.813496000	30.146970000
H	8.874700000	-2.077027000	29.263988000
C	10.445971000	-2.847187000	30.680938000
H	9.863480000	-3.739882000	30.995969000
H	11.119398000	-3.189639000	29.866067000
H	11.035964000	-2.455556000	31.530148000
O	8.580307000	-0.007974000	28.308818000
C	8.167736000	0.350719000	27.015297000
H	9.003079000	0.192677000	26.294243000
H	7.311714000	-0.285826000	26.687578000
H	7.849348000	1.417009000	26.938859000

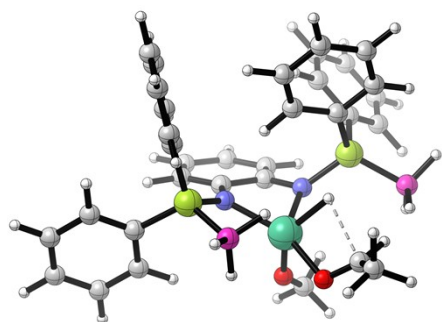
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P	9.023577000	3.526082000	30.589925000
P	4.900516000	0.194639000	29.829092000
N	8.048466000	2.751647000	29.419970000
N	5.977436000	1.309272000	29.218731000
C	7.036076000	3.325511000	28.630798000
C	5.849604000	2.520065000	28.534008000
C	4.742386000	2.959322000	27.780832000
H	3.848068000	2.323312000	27.702836000
C	4.802506000	4.196359000	27.116756000
H	3.936287000	4.541794000	26.532142000
C	5.974401000	4.973703000	27.174689000
H	6.029958000	5.927617000	26.629071000
C	7.088647000	4.540594000	27.912496000
H	8.005900000	5.141477000	27.927283000
C	8.895211000	5.340508000	30.284247000
C	9.951663000	6.019851000	29.643827000
H	10.867355000	5.467612000	29.386785000
C	9.826157000	7.383599000	29.332803000
H	10.655221000	7.907783000	28.832432000
C	8.648689000	8.077024000	29.660866000
H	8.549654000	9.144727000	29.411014000
C	7.600350000	7.407001000	30.315613000
H	6.678701000	7.947794000	30.580500000
C	7.723385000	6.046437000	30.630611000
H	6.899240000	5.523311000	31.137847000
C	8.119669000	3.411983000	32.190205000
C	8.781035000	3.778063000	33.378013000
H	9.834460000	4.094185000	33.340505000
C	8.094756000	3.730237000	34.603541000
H	8.616068000	4.009801000	35.532138000
C	6.749572000	3.325765000	34.645693000
H	6.215853000	3.286831000	35.608165000
C	6.087184000	2.965641000	33.458060000
H	5.037339000	2.640369000	33.481154000
C	6.770355000	3.007434000	32.234501000
H	6.269494000	2.695981000	31.306784000
C	3.768661000	-0.339745000	28.500259000
C	2.405763000	-0.606061000	28.734190000
H	1.981183000	-0.460452000	29.739454000
C	1.590858000	-1.044380000	27.677251000
H	0.525163000	-1.251377000	27.858747000
C	2.133895000	-1.213045000	26.392360000
H	1.492089000	-1.551612000	25.564763000
C	3.494996000	-0.943798000	26.160068000
H	3.918317000	-1.068926000	25.151905000
C	4.315879000	-0.508477000	27.209821000
H	5.378324000	-0.276012000	27.035793000
C	3.856426000	0.931305000	31.131054000
C	3.333357000	2.236269000	30.993930000
H	3.540849000	2.824457000	30.087708000
C	2.566002000	2.790221000	32.029228000
H	2.168167000	3.810617000	31.925626000

C	2.309782000	2.048328000	33.196874000
H	1.705844000	2.487068000	34.005970000
C	2.835398000	0.753241000	33.336939000
H	2.647046000	0.175497000	34.254579000
C	3.614899000	0.195658000	32.309887000
H	4.047750000	-0.809571000	32.422695000
B	10.870690000	2.980697000	30.566791000
H	10.915720000	1.760434000	30.722552000
H	11.420046000	3.610192000	31.472235000
H	11.261340000	3.314883000	29.446573000
B	6.206687000	-1.085386000	30.435302000
H	6.780975000	-1.404971000	29.387140000
H	5.793085000	-2.048047000	31.056733000
H	6.927121000	-0.364482000	31.157777000
O	9.316190000	-0.831161000	30.125441000
C	10.119894000	-0.786221000	31.061685000
H	10.077581000	0.080380000	31.767735000
C	11.155422000	-1.835147000	31.279557000
H	12.156289000	-1.351703000	31.257749000
H	11.042818000	-2.254262000	32.302628000
H	11.093810000	-2.637036000	30.520956000
O	8.607109000	0.582556000	27.907318000
C	9.539064000	1.243506000	27.097383000
H	10.557720000	0.812002000	27.223831000
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H	9.586476000	2.322678000	27.369321000

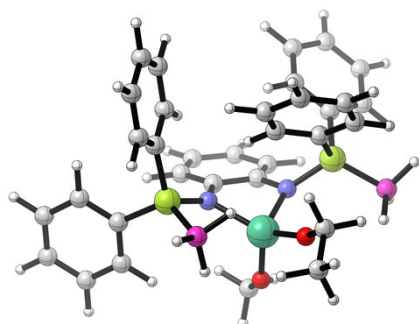
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P	4.573815000	0.287379000	29.866954000
N	7.951161000	2.426576000	28.951528000
N	5.729953000	1.198924000	29.084302000
C	6.951917000	2.954686000	28.108138000
C	5.687437000	2.278670000	28.200908000
C	4.591108000	2.700115000	27.420441000
H	3.631234000	2.168448000	27.491498000
C	4.742647000	3.783898000	26.539665000
H	3.885188000	4.114921000	25.934243000
C	5.989894000	4.422313000	26.410016000
H	6.114721000	5.250870000	25.696610000
C	7.090460000	4.006893000	27.177056000
H	8.063439000	4.496587000	27.051826000
C	8.917610000	5.073680000	29.377221000
C	9.987107000	5.592275000	28.618933000
H	10.875550000	4.967138000	28.446278000
C	9.908182000	6.889565000	28.087570000
H	10.745965000	7.288926000	27.495172000
C	8.765469000	7.676558000	28.313379000
H	8.704706000	8.692191000	27.893436000
C	7.704915000	7.168632000	29.084166000
H	6.811168000	7.784571000	29.268201000

C	7.781009000	5.873991000	29.617512000
H	6.946940000	5.476253000	30.214867000
C	8.137015000	3.503407000	31.594778000
C	8.856236000	4.045372000	32.678251000
H	9.913802000	4.321272000	32.547252000
C	8.222294000	4.222474000	33.919166000
H	8.788187000	4.639046000	34.766823000
C	6.872371000	3.865787000	34.080321000
H	6.378758000	4.004406000	35.054944000
C	6.154386000	3.327121000	32.998095000
H	5.100136000	3.038672000	33.118886000
C	6.785010000	3.144854000	31.758553000
H	6.239999000	2.692455000	30.918192000
C	3.355446000	-0.305681000	28.644092000
C	1.973828000	-0.345813000	28.913160000
H	1.590804000	0.011954000	29.880985000
C	1.088464000	-0.831546000	27.936484000
H	0.007850000	-0.861182000	28.145027000
C	1.579783000	-1.272188000	26.696107000
H	0.883187000	-1.646475000	25.930439000
C	2.960276000	-1.229483000	26.428318000
H	3.344836000	-1.567709000	25.454316000
C	3.851020000	-0.748823000	27.398208000
H	4.931686000	-0.693451000	27.189712000
C	3.645863000	1.302359000	31.065049000
C	3.277617000	2.632222000	30.764534000
H	3.542728000	3.072389000	29.792141000
C	2.595932000	3.398885000	31.720688000
H	2.320705000	4.438450000	31.489068000
C	2.271660000	2.844476000	32.972248000
H	1.737213000	3.450217000	33.720133000
C	2.641761000	1.523195000	33.274421000
H	2.399401000	1.092937000	34.257769000
C	3.334637000	0.752490000	32.326147000
H	3.647604000	-0.275077000	32.564411000
B	10.820107000	2.746403000	30.015634000
H	10.881983000	1.637880000	30.539139000
H	11.406372000	3.607932000	30.673309000
H	11.159778000	2.732133000	28.830883000
B	5.776428000	-1.023466000	30.603716000
H	6.611049000	-0.278481000	31.160690000
H	6.225630000	-1.557193000	29.585713000
H	5.317653000	-1.827280000	31.397549000
O	8.793973000	-1.179405000	30.039596000
C	9.575573000	-0.891770000	30.967533000
H	10.202229000	0.033657000	30.908190000
C	9.741229000	-1.768931000	32.161318000
H	10.815521000	-1.987810000	32.334413000
H	9.399735000	-1.187887000	33.046770000
H	9.147173000	-2.696273000	32.072933000
O	8.065195000	0.086671000	27.655810000
C	8.902213000	0.556999000	26.636084000
H	9.817862000	-0.070084000	26.556820000
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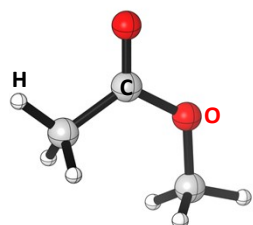
P



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P	9.113845000	3.435245000	29.825040000
P	4.657643000	0.392335000	29.752917000
N	8.080720000	2.431169000	28.875782000
N	5.857894000	1.195610000	28.920676000
C	7.140662000	2.900307000	27.932662000
C	5.871652000	2.230951000	27.982700000
C	4.830878000	2.615623000	27.113356000
H	3.864508000	2.092407000	27.154271000
C	5.046429000	3.654879000	26.191661000
H	4.231629000	3.957524000	25.516372000
C	6.300992000	4.287306000	26.112580000
H	6.471870000	5.084405000	25.373536000
C	7.347974000	3.906562000	26.968203000
H	8.329544000	4.392394000	26.896143000
C	8.628917000	5.165100000	29.442870000
C	9.587082000	6.039202000	28.893594000
H	10.612862000	5.677814000	28.727649000
C	9.224433000	7.354525000	28.557754000
H	9.975903000	8.036514000	28.131345000
C	7.907234000	7.796911000	28.764445000
H	7.622979000	8.825440000	28.494428000
C	6.951835000	6.927298000	29.321150000
H	5.920338000	7.273249000	29.487329000
C	7.311050000	5.617320000	29.665000000
H	6.562089000	4.939974000	30.100570000
C	8.433324000	3.242296000	31.525547000
C	9.261952000	3.501588000	32.634705000
H	10.309027000	3.797723000	32.472016000
C	8.752356000	3.360242000	33.936224000
H	9.405613000	3.555051000	34.800460000
C	7.420080000	2.959252000	34.137914000
H	7.028876000	2.840068000	35.160051000
C	6.590166000	2.702099000	33.032783000
H	5.546744000	2.383310000	33.177036000
C	7.096657000	2.845600000	31.732478000
H	6.454976000	2.620699000	30.868085000
C	3.431908000	-0.256249000	28.566919000
C	2.067587000	0.090723000	28.609961000
H	1.696350000	0.760374000	29.400731000
C	1.189859000	-0.411918000	27.634781000
H	0.124453000	-0.136907000	27.664838000
C	1.671782000	-1.256835000	26.621093000
H	0.982346000	-1.647339000	25.857061000
C	3.034713000	-1.604369000	26.579754000
H	3.412096000	-2.265772000	25.784707000
C	3.915880000	-1.107694000	27.549642000
H	4.985190000	-1.369568000	27.520956000
C	3.768698000	1.552347000	30.849226000
C	3.709171000	2.931204000	30.553079000
H	4.145645000	3.313071000	29.618053000
C	3.112450000	3.814923000	31.465171000
H	3.078126000	4.891107000	31.237287000

C	2.566995000	3.330597000	32.667174000
H	2.105078000	4.028440000	33.382064000
C	2.620858000	1.957249000	32.961465000
H	2.203199000	1.576999000	33.905963000
C	3.226670000	1.068089000	32.058818000
H	3.299985000	-0.003633000	32.300071000
B	10.987293000	3.105213000	29.662190000
H	11.136358000	1.927772000	29.972334000
H	11.521621000	3.900581000	30.439339000
H	11.238987000	3.342958000	28.479734000
B	5.800950000	-0.836915000	30.695929000
H	6.554404000	-0.010276000	31.241327000
H	6.380174000	-1.471598000	29.809079000
H	5.275312000	-1.543801000	31.537901000
O	8.947579000	0.267678000	30.691718000
C	9.343754000	0.098630000	32.031966000
H	10.313635000	0.630448000	32.157353000
C	9.478699000	-1.381900000	32.370088000
H	10.214904000	-1.871255000	31.701791000
H	9.815568000	-1.508697000	33.419279000
H	8.503653000	-1.896728000	32.251824000
O	8.171242000	-0.368058000	27.947172000
C	7.947250000	-0.185967000	26.571112000
H	8.652851000	0.568808000	26.159756000
H	8.110853000	-1.146720000	26.035110000
H	6.910034000	0.164732000	26.365186000

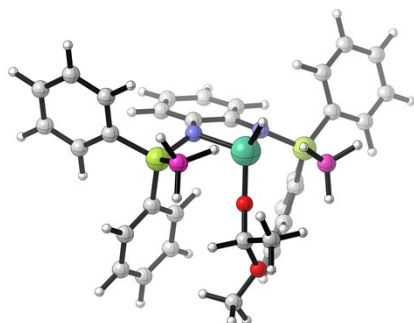
B



O	8.857386000	0.051745000	29.843501000
C	8.819225000	-0.597202000	28.821755000
C	9.993885000	-1.392941000	28.274686000
H	10.847090000	-1.266166000	28.963384000
H	9.751263000	-2.472042000	28.187061000
H	10.285980000	-1.039547000	27.264545000
O	7.652216000	-0.622724000	28.103000000
C	7.542361000	-1.371579000	26.894709000
H	8.246420000	-1.012646000	26.113518000
H	7.707255000	-2.458620000	27.056851000
H	6.508275000	-1.222172000	26.531856000

S14.2 XYZ coordinates of the molecules present in Figure S85

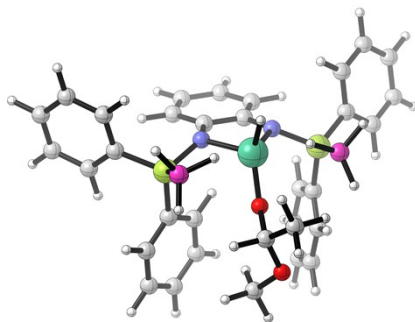
TS_{DE}



Ti	7.196798000	0.866345000	31.428401000
H	7.308270000	0.260506000	33.025507000
P	8.940360000	3.263302000	31.021940000
P	4.596893000	0.183458000	30.154375000
N	7.325905000	2.899732000	31.363579000
N	5.312465000	1.477913000	30.959360000
C	6.192164000	3.659573000	31.024626000
C	5.040663000	2.848172000	30.796707000
C	3.814103000	3.446550000	30.456731000
H	2.927924000	2.824928000	30.278953000
C	3.731652000	4.847004000	30.339234000
H	2.770799000	5.309370000	30.066988000
C	4.860720000	5.648333000	30.569676000
H	4.790166000	6.743560000	30.485012000
C	6.091836000	5.059429000	30.917030000
H	6.968065000	5.690613000	31.117818000
C	9.100503000	3.417208000	29.208489000
C	9.707102000	2.370097000	28.483134000
H	10.124861000	1.502018000	29.012525000
C	9.747659000	2.424957000	27.081042000
H	10.235503000	1.612472000	26.522894000
C	9.171313000	3.506807000	26.395569000
H	9.208157000	3.544907000	25.295400000
C	8.547920000	4.542351000	27.114651000
H	8.090295000	5.390614000	26.582802000
C	8.515719000	4.503835000	28.516698000
H	8.038607000	5.321318000	29.074179000
C	9.360949000	4.898787000	31.719828000
C	10.226273000	5.795109000	31.063023000
H	10.632400000	5.543751000	30.072146000
C	10.563705000	7.013292000	31.676403000
H	11.236577000	7.715777000	31.161021000
C	10.042633000	7.335496000	32.939910000
H	10.305813000	8.292838000	33.414643000
C	9.186774000	6.434809000	33.600137000
H	8.780504000	6.684398000	34.591566000
C	8.849481000	5.215968000	32.996457000
H	8.175427000	4.506057000	33.501935000
C	4.995704000	0.349417000	28.374974000
C	4.694500000	-0.708312000	27.491993000
H	4.213249000	-1.623013000	27.872423000
C	5.012399000	-0.596303000	26.129246000
H	4.775921000	-1.423885000	25.443043000
C	5.638022000	0.566738000	25.645526000
H	5.890804000	0.651356000	24.577333000
C	5.954900000	1.612973000	26.528381000
H	6.468197000	2.515227000	26.164829000
C	5.640515000	1.506435000	27.891960000
H	5.909265000	2.319661000	28.579916000
C	2.770455000	0.295522000	30.251303000
C	1.962002000	0.565429000	29.128482000
H	2.420443000	0.679712000	28.135400000
C	0.574034000	0.707514000	29.284655000
H	-0.054407000	0.919504000	28.406335000

C	-0.008426000	0.589015000	30.557743000
H	-1.096143000	0.709018000	30.679340000
C	0.797551000	0.318851000	31.677998000
H	0.342627000	0.224019000	32.675748000
C	2.183089000	0.166601000	31.527822000
H	2.817376000	-0.044436000	32.402045000
B	9.867080000	1.804203000	31.883089000
H	8.963302000	1.026222000	32.303954000
H	10.336322000	2.273984000	32.909794000
H	10.667423000	1.258609000	31.141569000
B	5.347884000	-1.334705000	31.079986000
H	6.273202000	-0.862488000	31.800321000
H	5.741763000	-2.188380000	30.302831000
H	4.507014000	-1.703891000	31.889726000
O	7.948349000	0.037879000	30.029065000
C	8.567571000	-1.187546000	29.640344000
H	7.724686000	-1.892958000	29.434453000
O	9.324696000	-1.000219000	28.477994000
C	8.527212000	-0.787101000	27.322994000
H	7.794530000	-1.615475000	27.177098000
H	7.966473000	0.167981000	27.384567000
H	9.208193000	-0.753687000	26.451137000
C	9.478019000	-1.720781000	30.733549000
H	8.894864000	-1.894143000	31.658744000
H	9.933087000	-2.675886000	30.408056000
H	10.276452000	-0.985914000	30.945624000

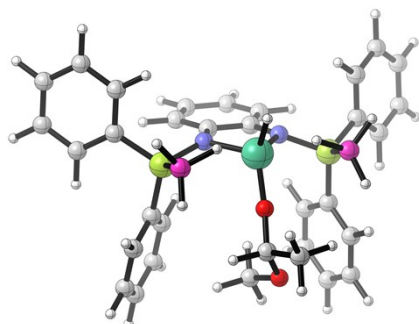
E



Ti	7.196798000	0.866345000	31.428401000
H	7.308270000	0.260506000	33.025507000
P	8.940360000	3.263302000	31.021940000
P	4.596893000	0.183458000	30.154375000
N	7.325905000	2.899732000	31.363579000
N	5.312465000	1.477913000	30.959360000
C	6.192164000	3.659573000	31.024626000
C	5.040663000	2.848172000	30.796707000
C	3.814103000	3.446550000	30.456731000
H	2.927924000	2.824928000	30.278953000
C	3.731652000	4.847004000	30.339234000
H	2.770799000	5.309370000	30.066988000
C	4.860720000	5.648333000	30.569676000
H	4.790166000	6.743560000	30.485012000
C	6.091836000	5.059429000	30.917030000
H	6.968065000	5.690613000	31.117818000
C	9.100503000	3.417208000	29.208489000
C	9.707102000	2.370097000	28.483134000
H	10.124861000	1.502018000	29.012525000
C	9.747659000	2.424957000	27.081042000
H	10.235503000	1.612472000	26.522894000
C	9.171313000	3.506807000	26.395569000
H	9.208157000	3.544907000	25.295400000
C	8.547920000	4.542351000	27.114651000
H	8.090295000	5.390614000	26.582802000
C	8.515719000	4.503835000	28.516698000

H	8.038607000	5.321318000	29.074179000
C	9.360949000	4.898787000	31.719828000
C	10.226273000	5.795109000	31.063023000
H	10.632400000	5.543751000	30.072146000
C	10.563705000	7.013292000	31.676403000
H	11.236577000	7.715777000	31.161021000
C	10.042633000	7.335496000	32.939910000
H	10.305813000	8.292838000	33.414643000
C	9.186774000	6.434809000	33.600137000
H	8.780504000	6.684398000	34.591566000
C	8.849481000	5.215968000	32.996457000
H	8.175427000	4.506057000	33.501935000
C	4.995704000	0.349417000	28.374974000
C	4.694500000	-0.708312000	27.491993000
H	4.213249000	-1.623013000	27.872423000
C	5.012399000	-0.596303000	26.129246000
H	4.775921000	-1.423885000	25.443043000
C	5.638022000	0.566738000	25.645526000
H	5.890804000	0.651356000	24.577333000
C	5.954900000	1.612973000	26.528381000
H	6.468197000	2.515227000	26.164829000
C	5.640515000	1.506435000	27.891960000
H	5.909265000	2.319661000	28.579916000
C	2.770455000	0.295522000	30.251303000
C	1.962002000	0.565429000	29.128482000
H	2.420443000	0.679712000	28.135400000
C	0.574034000	0.707514000	29.284655000
H	-0.054407000	0.919504000	28.406335000
C	-0.008426000	0.589015000	30.557743000
H	-1.096143000	0.709018000	30.679340000
C	0.797551000	0.318851000	31.677998000
H	0.342627000	0.224019000	32.675748000
C	2.183089000	0.166601000	31.527822000
H	2.817376000	-0.044436000	32.402045000
B	9.867080000	1.804203000	31.883089000
H	8.963302000	1.026222000	32.303954000
H	10.336322000	2.273984000	32.909794000
H	10.667423000	1.258609000	31.141569000
B	5.347884000	-1.334705000	31.079986000
H	6.273202000	-0.862488000	31.800321000
H	5.741763000	-2.188380000	30.302831000
H	4.507014000	-1.703891000	31.889726000
O	7.948349000	0.037879000	30.029065000
C	8.567571000	-1.187546000	29.640344000
H	7.724686000	-1.892958000	29.434453000
O	9.324696000	-1.000219000	28.477994000
C	8.527212000	-0.787101000	27.322994000
H	7.794530000	-1.615475000	27.177098000
H	7.966473000	0.167981000	27.384567000
H	9.208193000	-0.753687000	26.451137000
C	9.478019000	-1.720781000	30.733549000
H	8.894864000	-1.894143000	31.658744000
H	9.933087000	-2.675886000	30.408056000
H	10.276452000	-0.985914000	30.945624000

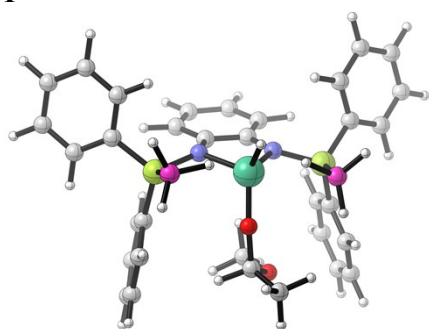
TS_{EF}



Ti	7.153455000	1.161232000	30.869563000
H	7.043359000	0.827047000	32.548053000
P	9.174296000	3.320388000	30.343148000
P	4.548253000	0.412270000	29.545902000
N	7.501433000	3.111073000	30.369097000
N	5.427121000	1.778057000	29.973874000
C	6.515099000	3.843821000	29.689989000
C	5.326698000	3.084603000	29.468409000
C	4.223519000	3.676123000	28.823473000
H	3.307991000	3.092935000	28.656128000
C	4.302595000	5.012824000	28.389457000
H	3.438075000	5.467672000	27.882717000
C	5.469876000	5.762216000	28.608636000
H	5.526360000	6.809122000	28.275253000
C	6.575128000	5.184914000	29.262660000
H	7.480711000	5.778466000	29.446571000
C	9.800954000	3.032689000	28.648595000
C	10.885292000	2.154365000	28.453555000
H	11.331560000	1.646254000	29.319479000
C	11.375533000	1.919506000	27.159276000
H	12.220332000	1.229753000	27.014691000
C	10.777615000	2.545129000	26.054497000
H	11.161988000	2.357206000	25.040215000
C	9.680032000	3.405063000	26.242057000
H	9.200985000	3.887912000	25.376857000
C	9.191570000	3.653065000	27.532597000
H	8.331779000	4.323341000	27.673036000
C	9.565693000	5.068415000	30.715833000
C	10.416965000	5.845986000	29.907407000
H	10.867351000	5.409754000	29.003640000
C	10.680225000	7.181854000	30.255010000
H	11.344758000	7.789507000	29.621613000
C	10.095510000	7.740783000	31.403104000
H	10.301668000	8.788234000	31.670712000
C	9.249023000	6.961646000	32.213275000
H	8.792175000	7.397532000	33.114421000
C	8.987311000	5.626961000	31.876159000
H	8.322273000	5.012498000	32.502917000
C	4.840629000	-0.007480000	27.788262000
C	4.761022000	-1.361093000	27.398000000
H	4.540732000	-2.133270000	28.150656000
C	4.976014000	-1.720548000	26.057496000
H	4.912524000	-2.777704000	25.758022000
C	5.285301000	-0.734511000	25.105452000
H	5.462905000	-1.018637000	24.056967000
C	5.379182000	0.612921000	25.495364000
H	5.632056000	1.386365000	24.754275000
C	5.156786000	0.980531000	26.831648000
H	5.238580000	2.035052000	27.131167000
C	2.761065000	0.795426000	29.652476000
C	1.866886000	0.555353000	28.591306000
H	2.235563000	0.122716000	27.649244000
C	0.508225000	0.882041000	28.736513000
H	-0.189770000	0.693728000	27.906402000

C	0.044299000	1.452066000	29.933659000
H	-1.019030000	1.715236000	30.042022000
C	0.938158000	1.689738000	30.994027000
H	0.575533000	2.137607000	31.931701000
C	2.293273000	1.358900000	30.858835000
H	2.999375000	1.549779000	31.681890000
B	9.744160000	2.070168000	31.697872000
H	8.698144000	1.443294000	32.041016000
H	10.007910000	2.734210000	32.691519000
H	10.626690000	1.320183000	31.317134000
B	5.191986000	-0.908235000	30.799571000
H	5.988026000	-0.273327000	31.555450000
H	5.718006000	-1.850368000	30.228432000
H	4.271430000	-1.194900000	31.552033000
O	8.047281000	0.034892000	29.848040000
C	8.646233000	-1.062253000	29.187877000
H	7.799582000	-1.741935000	28.910379000
O	9.318041000	-0.634746000	28.038098000
C	8.457291000	-0.058269000	27.067259000
H	7.646491000	-0.763153000	26.771604000
H	7.988976000	0.876515000	27.441746000
H	9.075310000	0.184211000	26.183822000
C	9.638954000	-1.745053000	30.111798000
H	9.120278000	-2.104288000	31.020156000
H	10.111521000	-2.602293000	29.594737000
H	10.418197000	-1.017889000	30.408955000

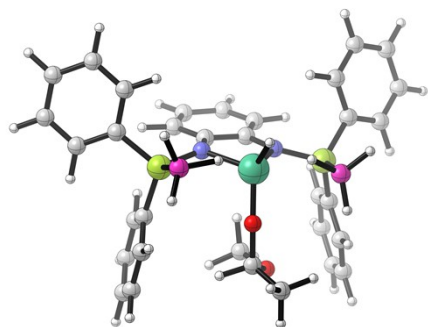
F



Ti	7.600924000	0.779210000	31.015301000
H	7.641099000	0.701172000	32.723595000
P	9.265432000	3.226492000	30.211726000
P	5.033431000	-0.489902000	30.011324000
N	7.684342000	2.636456000	30.164472000
N	5.786966000	1.015020000	30.083610000
C	6.605639000	3.109932000	29.403178000
C	5.535456000	2.166769000	29.326099000
C	4.374671000	2.489262000	28.594689000
H	3.540637000	1.776168000	28.541812000
C	4.267348000	3.741559000	27.960970000
H	3.355193000	3.982712000	27.394659000
C	5.302546000	4.683500000	28.070325000
H	5.207036000	5.672137000	27.597196000
C	6.467050000	4.373455000	28.797438000
H	7.257755000	5.125858000	28.921224000
C	10.058896000	3.159122000	28.562568000
C	11.209318000	2.359339000	28.403891000
H	11.610757000	1.817324000	29.270085000
C	11.821733000	2.243572000	27.146366000
H	12.717966000	1.615733000	27.034652000
C	11.283769000	2.911867000	26.035654000
H	11.760123000	2.813566000	25.048018000
C	10.134492000	3.708839000	26.185730000
H	9.706532000	4.232575000	25.317599000

C	9.525780000	3.838877000	27.442129000
H	8.626003000	4.458479000	27.543108000
C	9.185929000	5.001940000	30.649186000
C	10.031712000	5.964614000	30.064510000
H	10.747368000	5.667245000	29.282933000
C	9.951752000	7.305708000	30.475918000
H	10.610519000	8.057823000	30.015685000
C	9.033061000	7.685996000	31.467887000
H	8.971569000	8.737684000	31.787087000
C	8.191973000	6.723408000	32.054725000
H	7.471344000	7.019820000	32.832369000
C	8.267971000	5.383505000	31.650521000
H	7.607633000	4.624182000	32.097937000
C	5.433424000	-1.283373000	28.411026000
C	6.063806000	-2.544695000	28.407815000
H	6.272909000	-3.041612000	29.366288000
C	6.429429000	-3.147930000	27.193118000
H	6.918049000	-4.133675000	27.198676000
C	6.174756000	-2.492995000	25.977100000
H	6.465332000	-2.963566000	25.025678000
C	5.551431000	-1.232092000	25.976168000
H	5.357592000	-0.713020000	25.025363000
C	5.177614000	-0.627217000	27.184965000
H	4.703705000	0.363907000	27.174583000
C	3.217925000	-0.262249000	30.008707000
C	2.366982000	-0.927631000	29.105360000
H	2.789702000	-1.601250000	28.344493000
C	0.978427000	-0.721121000	29.172087000
H	0.315135000	-1.241743000	28.464500000
C	0.440667000	0.148628000	30.134743000
H	-0.646798000	0.315553000	30.179867000
C	1.290618000	0.807165000	31.042185000
H	0.869641000	1.487948000	31.797962000
C	2.675210000	0.599654000	30.986062000
H	3.347403000	1.115874000	31.688959000
B	10.053671000	2.094659000	31.562591000
H	9.057458000	1.509694000	32.089833000
H	10.452510000	2.805070000	32.474725000
H	10.875474000	1.316927000	31.113528000
B	5.721875000	-1.346719000	31.593432000
H	6.615235000	-0.565724000	32.042708000
H	6.164310000	-2.466134000	31.395608000
H	4.832482000	-1.269848000	32.431303000
O	8.552591000	-0.466361000	30.190429000
C	9.315011000	-1.110491000	29.188006000
H	8.645207000	-1.891940000	28.749020000
O	9.710592000	-0.209801000	28.192859000
C	8.641082000	0.319887000	27.422123000
H	8.052455000	-0.488702000	26.934178000
H	7.948357000	0.933249000	28.040041000
H	9.092274000	0.970849000	26.650844000
C	10.559352000	-1.720573000	29.810979000
H	10.272332000	-2.440761000	30.599810000
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H	11.167803000	-0.915670000	30.266893000

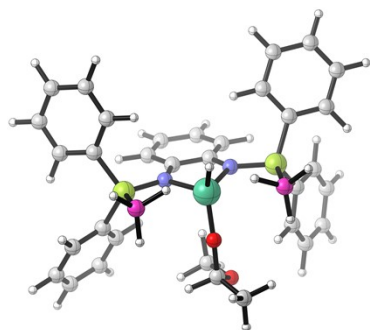
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Ti	7.635905000	0.773861000	30.991395000
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P	5.045429000	-0.497041000	30.028346000
N	7.711840000	2.630785000	30.131477000
N	5.823170000	0.996565000	30.049794000
C	6.646283000	3.079563000	29.337912000
C	5.581082000	2.130085000	29.262612000
C	4.432956000	2.430971000	28.502790000
H	3.601034000	1.715303000	28.453714000
C	4.332939000	3.666716000	27.836448000
H	3.430265000	3.890666000	27.248232000
C	5.363111000	4.614274000	27.941338000
H	5.273061000	5.591093000	27.443176000
C	6.514326000	4.326065000	28.697669000
H	7.295845000	5.086846000	28.821550000
C	10.103245000	3.235230000	28.580984000
C	11.141692000	2.305612000	28.366457000
H	11.456960000	1.653848000	29.190590000
C	11.749354000	2.202945000	27.105546000
H	12.554393000	1.469479000	26.949576000
C	11.319689000	3.018326000	26.047024000
H	11.790492000	2.930415000	25.055781000
C	10.290341000	3.954245000	26.255429000
H	9.953910000	4.600711000	25.430670000
C	9.688515000	4.069201000	27.516355000
H	8.896333000	4.813164000	27.667626000
C	9.154293000	5.016937000	30.690218000
C	10.078098000	5.981011000	30.239962000
H	10.879424000	5.692590000	29.542846000
C	9.968827000	7.311031000	30.678519000
H	10.688545000	8.064058000	30.322722000
C	8.943267000	7.679486000	31.565456000
H	8.858376000	8.722929000	31.905402000
C	8.025994000	6.715380000	32.020667000
H	7.222195000	7.002402000	32.715942000
C	8.130817000	5.385836000	31.588314000
H	7.414728000	4.624149000	31.933688000
C	5.413302000	-1.349803000	28.450426000
C	6.049863000	-2.607768000	28.481910000
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C	6.398877000	-3.252534000	27.283789000
H	6.891838000	-4.235609000	27.317002000
C	6.122246000	-2.642784000	26.049292000
H	6.400546000	-3.145750000	25.110867000
C	5.490936000	-1.386461000	26.013347000
H	5.277910000	-0.903286000	25.047848000
C	5.132373000	-0.741086000	27.205694000
H	4.651837000	0.245814000	27.167474000
C	3.234644000	-0.236998000	30.037068000
C	2.359486000	-0.956770000	29.201102000
H	2.760164000	-1.690741000	28.485268000
C	0.974769000	-0.729101000	29.278017000
H	0.292360000	-1.292573000	28.623439000

C	0.465211000	0.215952000	30.183287000
H	-0.619357000	0.398541000	30.236247000
C	1.339500000	0.929689000	31.023195000
H	0.940406000	1.670495000	31.733001000
C	2.720393000	0.701517000	30.957399000
H	3.412212000	1.260581000	31.606506000
B	10.068392000	2.105494000	31.553334000
H	9.070990000	1.520052000	32.080564000
H	10.477167000	2.801236000	32.471909000
H	10.884230000	1.327712000	31.091132000
B	5.737980000	-1.318520000	31.625816000
H	6.649376000	-0.541420000	32.047472000
H	6.164787000	-2.448574000	31.455893000
H	4.860050000	-1.207516000	32.471870000
O	8.573640000	-0.476818000	30.155824000
C	9.275578000	-1.114582000	29.105314000
H	8.570838000	-1.871485000	28.678110000
O	9.651327000	-0.202427000	28.112279000
C	8.565075000	0.372086000	27.397932000
H	7.959724000	-0.407465000	26.883354000
H	7.894272000	0.955803000	28.065415000
H	8.999591000	1.061007000	26.650019000
C	10.529726000	-1.768546000	29.660850000
H	10.257334000	-2.500683000	30.443893000
H	11.081177000	-2.281347000	28.848838000
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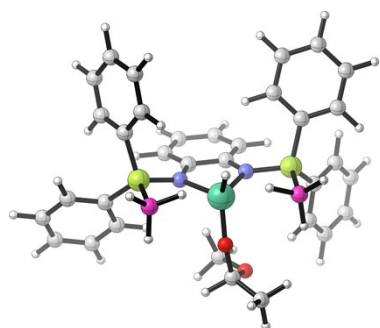
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P	-2.608961000	-1.272667000	0.350953000
N	1.216794000	0.220384000	0.696172000
N	-1.138585000	-0.463829000	0.318299000
C	0.514571000	1.150827000	-0.083287000
C	-0.849046000	0.775007000	-0.269790000
C	-1.726059000	1.633846000	-0.957834000
H	-2.785663000	1.365373000	-1.070189000
C	-1.240443000	2.842951000	-1.491197000
H	-1.929490000	3.511862000	-2.028593000
C	0.109804000	3.197024000	-1.335799000
H	0.485761000	4.141744000	-1.755756000
C	0.990619000	2.356620000	-0.629010000
H	2.040312000	2.646112000	-0.491850000
C	3.855462000	0.504504000	-0.387683000
C	3.875344000	-0.569117000	-1.303464000
H	3.333263000	-1.502379000	-1.084900000
C	4.575504000	-0.439010000	-2.511928000
H	4.584946000	-1.279510000	-3.223428000
C	5.263424000	0.750641000	-2.809415000
H	5.814074000	0.846963000	-3.757788000
C	5.246933000	1.817660000	-1.895284000
H	5.781392000	2.752022000	-2.125127000

C	4.541378000	1.699080000	-0.687131000
H	4.520359000	2.540771000	0.022191000
C	3.139150000	1.723966000	2.179539000
C	4.443047000	1.984546000	2.652904000
H	5.279423000	1.333871000	2.352393000
C	4.671232000	3.068298000	3.513989000
H	5.688780000	3.269984000	3.881400000
C	3.600425000	3.887382000	3.913926000
H	3.782259000	4.737383000	4.589531000
C	2.299332000	3.615387000	3.459708000
H	1.458397000	4.248862000	3.779946000
C	2.064081000	2.532745000	2.596786000
H	1.046560000	2.311340000	2.244125000
C	-3.180591000	-1.735041000	-1.321056000
C	-4.212366000	-2.694228000	-1.415896000
H	-4.652080000	-3.120519000	-0.500679000
C	-4.665769000	-3.114772000	-2.675020000
H	-5.471844000	-3.861230000	-2.745363000
C	-4.082005000	-2.594522000	-3.843228000
H	-4.434390000	-2.930023000	-4.830258000
C	-3.043393000	-1.653535000	-3.749862000
H	-2.579202000	-1.249917000	-4.662284000
C	-2.591156000	-1.220929000	-2.492527000
H	-1.780365000	-0.482295000	-2.423010000
C	-3.857503000	-0.097243000	0.998098000
C	-5.062000000	0.199620000	0.331713000
H	-5.294744000	-0.284652000	-0.628363000
C	-5.959266000	1.125045000	0.890240000
H	-6.898792000	1.358141000	0.366450000
C	-5.656584000	1.754809000	2.108165000
H	-6.360984000	2.481422000	2.541459000
C	-4.453495000	1.458550000	2.773467000
H	-4.214651000	1.950226000	3.728390000
C	-3.554595000	0.534727000	2.222715000
H	-2.607183000	0.305567000	2.736278000
B	3.072306000	-1.431475000	1.997445000
H	1.912286000	-1.628202000	2.480580000
H	3.777610000	-1.303884000	2.987473000
H	3.437653000	-2.263856000	1.185715000
B	-2.200681000	-2.798789000	1.450742000
H	-1.229772000	-2.380084000	2.154914000
H	-1.926014000	-3.738783000	0.722421000
H	-3.088544000	-2.996399000	2.267517000
O	0.779263000	-2.954188000	0.328677000
C	1.099829000	-3.737620000	-0.794622000
H	0.128431000	-4.138763000	-1.183970000
C	2.047386000	-4.855033000	-0.392297000
H	1.574813000	-5.483062000	0.386237000
H	2.293750000	-5.480647000	-1.271831000
H	2.976724000	-4.417167000	0.019556000
O	1.722263000	-2.967443000	-1.795983000
C	0.877771000	-1.982300000	-2.374814000
H	-0.031489000	-2.444232000	-2.823999000
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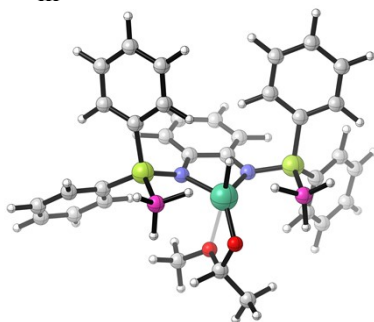
H



Ti	0.767327000	-1.342872000	1.051306000
H	0.619440000	-1.589429000	2.740618000
P	2.246358000	1.375042000	1.115338000
P	-2.117241000	-2.149591000	0.216088000
N	0.926240000	0.586930000	0.425675000
N	-0.932217000	-0.987457000	-0.060166000
C	-0.007940000	1.131429000	-0.468893000
C	-1.089263000	0.236894000	-0.723871000
C	-2.145990000	0.637510000	-1.562590000
H	-2.983203000	-0.045319000	-1.758401000
C	-2.121231000	1.914684000	-2.154471000
H	-2.950525000	2.222711000	-2.809140000
C	-1.048235000	2.788547000	-1.914252000
H	-1.031565000	3.785020000	-2.380164000
C	0.011446000	2.402487000	-1.071199000
H	0.842835000	3.092177000	-0.876228000
C	3.230712000	2.190258000	-0.197042000
C	3.784071000	1.342565000	-1.181469000
H	3.623181000	0.252016000	-1.136037000
C	4.526256000	1.896489000	-2.235575000
H	4.954068000	1.233560000	-3.003418000
C	4.727256000	3.286219000	-2.310180000
H	5.312762000	3.715545000	-3.138082000
C	4.179002000	4.127694000	-1.328019000
H	4.333542000	5.216446000	-1.382952000
C	3.426994000	3.583926000	-0.273737000
H	2.985070000	4.248039000	0.484200000
C	1.618780000	2.702594000	2.202334000
C	2.534517000	3.460146000	2.963471000
H	3.615890000	3.267421000	2.878414000
C	2.066052000	4.451697000	3.838737000
H	2.781876000	5.042022000	4.430932000
C	0.684748000	4.682316000	3.966370000
H	0.318255000	5.460796000	4.653452000
C	-0.227657000	3.912325000	3.226625000
H	-1.310074000	4.082253000	3.333489000
C	0.234047000	2.919490000	2.347827000
H	-0.479631000	2.309373000	1.775344000
C	-2.826231000	-2.760439000	-1.350419000
C	-4.017970000	-3.515579000	-1.346987000
H	-4.567579000	-3.677027000	-0.406742000
C	-4.502385000	-4.063905000	-2.544678000
H	-5.435374000	-4.647590000	-2.539946000
C	-3.797503000	-3.869083000	-3.745182000
H	-4.180338000	-4.297726000	-4.683610000
C	-2.601403000	-3.131243000	-3.746008000
H	-2.045444000	-2.981424000	-4.683927000
C	-2.111893000	-2.580856000	-2.552107000
H	-1.175322000	-2.004554000	-2.544941000
C	-3.467662000	-1.313224000	1.124665000
C	-4.638872000	-0.825140000	0.511608000
H	-4.824417000	-1.016858000	-0.555638000
C	-5.573367000	-0.096543000	1.265308000
H	-6.486841000	0.283245000	0.782999000

C	-5.340013000	0.152436000	2.627670000
H	-6.074573000	0.724290000	3.215565000
C	-4.169739000	-0.329261000	3.241253000
H	-3.984578000	-0.135811000	4.308798000
C	-3.235605000	-1.061449000	2.494708000
H	-2.316120000	-1.436588000	2.971942000
B	3.129087000	-0.068368000	2.016561000
H	2.139571000	-0.779921000	2.377898000
H	3.626490000	0.307749000	3.067336000
H	3.882129000	-0.607346000	1.225176000
B	-1.116251000	-3.465713000	1.183038000
H	-0.347343000	-2.748156000	1.895786000
H	-0.535595000	-4.143774000	0.350677000
H	-1.805367000	-4.069324000	1.992460000
O	1.846291000	-2.466178000	0.193049000
C	2.672124000	-2.815257000	-0.892622000
H	2.140071000	-3.633923000	-1.442483000
C	4.029306000	-3.275571000	-0.387301000
H	3.900555000	-4.131838000	0.301223000
H	4.669290000	-3.578025000	-1.238544000
H	4.514342000	-2.445579000	0.161837000
O	2.870094000	-1.722736000	-1.761792000
C	1.717242000	-1.352734000	-2.506647000
H	1.442593000	-2.144664000	-3.242139000
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TS_{III}

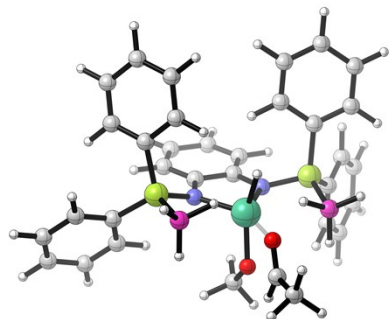


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P	-1.947567000	-2.017659000	0.073754000
N	1.173870000	0.609817000	0.196595000
N	-0.749831000	-0.899952000	-0.278683000
C	0.208368000	1.213479000	-0.625865000
C	-0.917580000	0.366613000	-0.848491000
C	-2.038448000	0.863313000	-1.540182000
H	-2.935047000	0.238683000	-1.659246000
C	-2.017136000	2.174334000	-2.054751000
H	-2.896571000	2.556459000	-2.594831000
C	-0.888254000	2.990027000	-1.875292000
H	-0.873899000	4.011510000	-2.283242000
C	0.225343000	2.516923000	-1.154527000
H	1.093353000	3.167557000	-0.985165000
C	3.385278000	2.375575000	-0.105376000
C	3.898642000	1.625902000	-1.187024000
H	3.641596000	0.558200000	-1.275680000
C	4.702659000	2.250009000	-2.150692000
H	5.097159000	1.665261000	-2.995778000
C	5.002291000	3.619863000	-2.040187000
H	5.635416000	4.107815000	-2.797318000
C	4.487385000	4.366860000	-0.968169000
H	4.714993000	5.440543000	-0.883340000

C	3.675143000	3.749420000	-0.002156000
H	3.254314000	4.343519000	0.822408000
C	1.494878000	2.615796000	2.176707000
C	2.248687000	3.431274000	3.048527000
H	3.349593000	3.390506000	3.030994000
C	1.596119000	4.272855000	3.963391000
H	2.188445000	4.906358000	4.641414000
C	0.191861000	4.291314000	4.024952000
H	-0.319140000	4.948942000	4.745117000
C	-0.558149000	3.456404000	3.179490000
H	-1.658082000	3.452972000	3.234241000
C	0.087313000	2.615306000	2.260140000
H	-0.502074000	1.950729000	1.613970000
C	-2.780707000	-2.693816000	-1.405172000
C	-3.698116000	-3.751431000	-1.220382000
H	-3.926635000	-4.109597000	-0.204258000
C	-4.308290000	-4.353569000	-2.330738000
H	-5.022976000	-5.177318000	-2.180941000
C	-3.997721000	-3.914154000	-3.629734000
H	-4.475098000	-4.389544000	-4.499928000
C	-3.072646000	-2.873318000	-3.815933000
H	-2.823666000	-2.530764000	-4.831799000
C	-2.462404000	-2.263702000	-2.708005000
H	-1.740745000	-1.447218000	-2.852298000
C	-3.225534000	-1.101470000	1.013824000
C	-4.552934000	-0.942902000	0.571457000
H	-4.886640000	-1.428825000	-0.357636000
C	-5.445982000	-0.151113000	1.312535000
H	-6.481755000	-0.023565000	0.962686000
C	-5.016441000	0.484481000	2.488783000
H	-5.718481000	1.106396000	3.065308000
C	-3.689299000	0.328736000	2.928433000
H	-3.347423000	0.824615000	3.849487000
C	-2.792073000	-0.460033000	2.195217000
H	-1.742975000	-0.569456000	2.521720000
B	3.223214000	0.018392000	2.023939000
H	2.196517000	-0.653522000	2.340443000
H	3.683883000	0.436143000	3.076075000
H	3.998429000	-0.535171000	1.263864000
B	-0.925025000	-3.344596000	1.008342000
H	-0.225737000	-2.631723000	1.775644000
H	-0.298700000	-3.955432000	0.151014000
H	-1.610560000	-4.038065000	1.743900000
O	2.240418000	-2.650262000	0.857693000
C	2.414997000	-3.156993000	-0.408216000
H	1.902716000	-4.146401000	-0.524752000
C	3.881185000	-3.236401000	-0.804905000
H	4.410761000	-3.947897000	-0.142082000
H	3.991557000	-3.582449000	-1.852576000
H	4.345942000	-2.237284000	-0.694543000
O	1.708533000	-2.190319000	-1.243624000
C	1.039836000	-2.692611000	-2.388780000
H	1.756122000	-3.158714000	-3.102084000
H	0.261024000	-3.437530000	-2.111848000
H	0.557732000	-1.828334000	-2.881155000

S14.3 XYZ coordinates of the molecules present in Figure S86

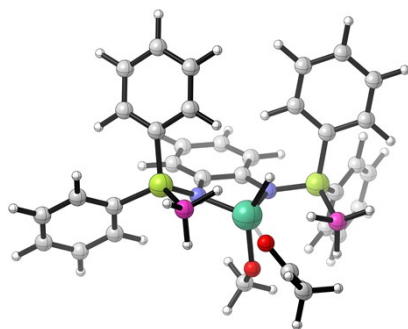
TS_{JK}



Ti	7.855550000	0.878201000	29.883008000
H	7.713004000	0.846268000	31.620496000
P	9.063647000	3.693113000	30.278716000
P	4.919557000	-0.018640000	29.549733000
N	7.776845000	2.892539000	29.542399000
N	5.971654000	1.236420000	29.153325000
C	6.624518000	3.485162000	29.006085000
C	5.583597000	2.533918000	28.794763000
C	4.331645000	2.956922000	28.310427000
H	3.521964000	2.229942000	28.161662000
C	4.120208000	4.317376000	28.020828000
H	3.140865000	4.644268000	27.640045000
C	5.149242000	5.252392000	28.217978000
H	4.980711000	6.315823000	27.989950000
C	6.401108000	4.844013000	28.713947000
H	7.195119000	5.581964000	28.881667000
C	9.665910000	5.043281000	29.194834000
C	10.204282000	4.650943000	27.950413000
H	10.269575000	3.580428000	27.701433000
C	10.644336000	5.621039000	27.038527000
H	11.056729000	5.309645000	26.066913000
C	10.560177000	6.985854000	27.365529000
H	10.908033000	7.745932000	26.649497000
C	10.029764000	7.378659000	28.605946000
H	9.958879000	8.446832000	28.863348000
C	9.578352000	6.412204000	29.519075000
H	9.141540000	6.723339000	30.479355000
C	8.418240000	4.469887000	31.802083000
C	9.272998000	5.221683000	32.635806000
H	10.322806000	5.387987000	32.347211000
C	8.789527000	5.743101000	33.846006000
H	9.459444000	6.325803000	34.496916000
C	7.457973000	5.508691000	34.232230000
H	7.082410000	5.915732000	35.183278000
C	6.613014000	4.742951000	33.411279000
H	5.573413000	4.544450000	33.712759000
C	7.090016000	4.217473000	32.200957000
H	6.437650000	3.598548000	31.569064000
C	3.901641000	-0.504266000	28.115820000
C	2.837445000	-1.416833000	28.278236000
H	2.571418000	-1.782830000	29.282003000
C	2.123318000	-1.865451000	27.156485000
H	1.290473000	-2.573496000	27.286988000
C	2.474382000	-1.416876000	25.871360000
H	1.912845000	-1.770416000	24.993432000
C	3.546534000	-0.523261000	25.707484000
H	3.827288000	-0.175981000	24.701648000
C	4.263510000	-0.068953000	26.824925000
H	5.106907000	0.627972000	26.704986000
C	3.806456000	0.686583000	30.822611000
C	2.445754000	0.979191000	30.611711000
H	1.965590000	0.714034000	29.658288000
C	1.703559000	1.623529000	31.615904000
H	0.641526000	1.856294000	31.444644000

C	2.318080000	1.981622000	32.826542000
H	1.734982000	2.488545000	33.610918000
C	3.679779000	1.696333000	33.035161000
H	4.165794000	1.977162000	33.982136000
C	4.426513000	1.051654000	32.039142000
H	5.501527000	0.851984000	32.190101000
B	10.276946000	2.244012000	30.557846000
H	9.448838000	1.411669000	31.012024000
H	11.050756000	2.461771000	31.478367000
H	10.775536000	1.950156000	29.481614000
B	6.166863000	-1.343438000	30.136155000
H	6.926072000	-0.614766000	30.834632000
H	6.671735000	-1.817127000	29.130522000
H	5.682119000	-2.138869000	30.928331000
O	9.240253000	-0.862429000	30.785945000
C	9.934011000	-1.606760000	30.099446000
H	9.932013000	-1.462250000	28.987724000
C	10.777508000	-2.692964000	30.688311000
H	10.469896000	-3.668465000	30.253678000
H	11.836293000	-2.540075000	30.386026000
H	10.690639000	-2.718857000	31.790578000
O	8.701801000	0.147651000	28.392885000
C	8.420443000	0.600890000	27.093863000
H	9.362646000	0.687099000	26.503848000
H	7.753236000	-0.120879000	26.565326000
H	7.919382000	1.597062000	27.082737000

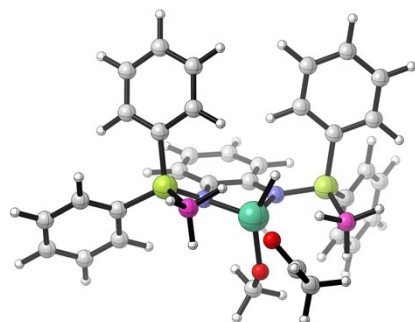
K



Ti	7.772514000	0.695255000	29.780753000
H	7.858449000	0.893477000	31.511303000
P	9.069195000	3.520925000	30.228994000
P	4.808255000	-0.030037000	29.537918000
N	7.758918000	2.734508000	29.505579000
N	5.913048000	1.129416000	29.014708000
C	6.631207000	3.366233000	28.961219000
C	5.579034000	2.446595000	28.677299000
C	4.351147000	2.905200000	28.164071000
H	3.540889000	2.191502000	27.960645000
C	4.165907000	4.277332000	27.921390000
H	3.206048000	4.634177000	27.518538000
C	5.200258000	5.186842000	28.198793000
H	5.054119000	6.262237000	28.015285000
C	6.427671000	4.741630000	28.720345000
H	7.215410000	5.467053000	28.954151000
C	9.577347000	4.949543000	29.196602000
C	9.901301000	4.677520000	27.850241000
H	9.826402000	3.646840000	27.471571000
C	10.295793000	5.718936000	26.999066000
H	10.539658000	5.501956000	25.948016000
C	10.380077000	7.035406000	27.486606000
H	10.691551000	7.851884000	26.817423000
C	10.063563000	7.307378000	28.827851000
H	10.126255000	8.337064000	29.212142000

C	9.658293000	6.269502000	29.683040000
H	9.387478000	6.488070000	30.726559000
C	8.468127000	4.218261000	31.809619000
C	9.394111000	4.752409000	32.730201000
H	10.468525000	4.759264000	32.487561000
C	8.948234000	5.255381000	33.962996000
H	9.673888000	5.667904000	34.680480000
C	7.580352000	5.218106000	34.284478000
H	7.231530000	5.610068000	35.252076000
C	6.660569000	4.668216000	33.374880000
H	5.589009000	4.628318000	33.624547000
C	7.099373000	4.162731000	32.141656000
H	6.381135000	3.719574000	31.438351000
C	3.761347000	-0.607869000	28.162171000
C	2.676521000	-1.477593000	28.404752000
H	2.416710000	-1.763930000	29.435816000
C	1.932465000	-1.983044000	27.327794000
H	1.082429000	-2.655767000	27.519437000
C	2.275074000	-1.635095000	26.009291000
H	1.689647000	-2.032934000	25.166685000
C	3.368691000	-0.786234000	25.767008000
H	3.643003000	-0.519732000	24.734993000
C	4.115117000	-0.274234000	26.839389000
H	4.976997000	0.387077000	26.663069000
C	3.736819000	0.826834000	30.748917000
C	2.380851000	1.130880000	30.524114000
H	1.883661000	0.786213000	29.605445000
C	1.666142000	1.887352000	31.467911000
H	0.607816000	2.128091000	31.285502000
C	2.303407000	2.346379000	32.631660000
H	1.741480000	2.940250000	33.369120000
C	3.661279000	2.052342000	32.852190000
H	4.166371000	2.412223000	33.761344000
C	4.380861000	1.297902000	31.915565000
H	5.451831000	1.091535000	32.076434000
B	10.405062000	2.167294000	30.389475000
H	9.652015000	1.235619000	30.732355000
H	11.167448000	2.415158000	31.315645000
H	10.918363000	2.019034000	29.287523000
B	6.077294000	-1.272842000	30.230889000
H	6.685369000	-0.506986000	31.023692000
H	6.740905000	-1.563395000	29.237096000
H	5.651487000	-2.218979000	30.867465000
O	8.973870000	-1.023900000	30.610508000
C	10.137549000	-1.239359000	30.264169000
H	10.604811000	-0.582556000	29.490236000
C	10.947716000	-2.354544000	30.838284000
H	11.328738000	-2.997481000	30.016324000
H	11.844575000	-1.926605000	31.336447000
H	10.358568000	-2.952199000	31.558265000
O	8.805617000	0.187748000	28.318797000
C	8.718609000	0.809109000	27.065609000
H	9.604683000	1.466400000	26.894750000
H	8.710818000	0.041314000	26.257505000
H	7.804332000	1.437712000	26.950280000

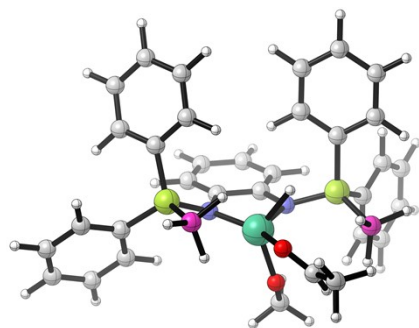
TS_{KL}



Ti	7.610164000	0.793741000	29.734699000
H	7.717377000	0.977545000	31.466019000
P	9.038290000	3.549760000	30.216068000
P	4.615653000	0.203268000	29.529078000
N	7.690584000	2.835395000	29.485549000
N	5.761391000	1.325399000	29.013091000
C	6.583802000	3.525995000	28.970675000
C	5.482945000	2.661001000	28.699160000
C	4.267892000	3.182782000	28.216784000
H	3.421176000	2.509738000	28.023776000
C	4.143548000	4.564674000	27.991157000
H	3.193638000	4.970810000	27.612037000
C	5.226376000	5.420481000	28.254541000
H	5.128909000	6.503383000	28.083459000
C	6.441563000	4.911842000	28.746052000
H	7.268074000	5.596662000	28.967738000
C	9.605733000	4.974862000	29.208294000
C	9.942605000	4.708258000	27.864157000
H	9.847429000	3.683501000	27.474078000
C	10.377369000	5.747141000	27.029489000
H	10.630885000	5.534259000	25.979914000
C	10.490014000	7.055732000	27.532021000
H	10.832866000	7.870340000	26.876022000
C	10.161860000	7.322314000	28.871597000
H	10.247278000	8.345830000	29.267763000
C	9.715978000	6.287215000	29.709715000
H	9.436144000	6.502335000	30.751521000
C	8.473121000	4.245326000	31.810629000
C	9.424525000	4.739974000	32.727309000
H	10.496047000	4.716224000	32.473205000
C	9.007034000	5.243911000	33.969511000
H	9.752267000	5.626307000	34.683556000
C	7.641727000	5.247391000	34.303809000
H	7.314556000	5.641061000	35.278237000
C	6.696155000	4.736398000	33.398039000
H	5.626257000	4.729544000	33.657841000
C	7.106608000	4.229339000	32.155651000
H	6.368479000	3.814198000	31.455712000
C	3.525004000	-0.302080000	28.158913000
C	2.413348000	-1.137018000	28.402375000
H	2.164201000	-1.440818000	29.431144000
C	1.628727000	-1.585760000	27.329087000
H	0.757793000	-2.230844000	27.521607000
C	1.957321000	-1.216398000	26.012838000
H	1.340021000	-1.569856000	25.173128000
C	3.077328000	-0.403191000	25.768864000
H	3.340344000	-0.119911000	24.738411000
C	3.864580000	0.052093000	26.837835000
H	4.746582000	0.685662000	26.660117000
C	3.596220000	1.076234000	30.773200000
C	2.249452000	1.435358000	30.575685000
H	1.725184000	1.126765000	29.659328000
C	1.578391000	2.200096000	31.544587000
H	0.527454000	2.484043000	31.383286000

C	2.249992000	2.612251000	32.706554000
H	1.722879000	3.213494000	33.463462000
C	3.598353000	2.261757000	32.900565000
H	4.130290000	2.583906000	33.808594000
C	4.274626000	1.498914000	31.938791000
H	5.338755000	1.248738000	32.079776000
B	10.322733000	2.143925000	30.345763000
H	9.546253000	1.233071000	30.686625000
H	11.108518000	2.357809000	31.261404000
H	10.817114000	1.992973000	29.235174000
B	5.844003000	-1.103900000	30.178112000
H	6.488537000	-0.380578000	30.980298000
H	6.486871000	-1.392982000	29.169763000
H	5.390181000	-2.050079000	30.794545000
O	8.746660000	-0.982876000	30.530690000
C	9.897420000	-1.242375000	30.171439000
H	10.386828000	-0.594153000	29.404191000
C	10.663031000	-2.400076000	30.722240000
H	11.011377000	-3.044943000	29.887403000
H	11.580230000	-2.017854000	31.220496000
H	10.054131000	-2.983931000	31.437057000
O	8.615718000	0.274604000	28.257956000
C	8.532811000	0.911400000	27.012120000
H	9.419733000	1.569145000	26.850047000
H	8.524098000	0.152767000	26.195540000
H	7.620548000	1.543782000	26.902819000

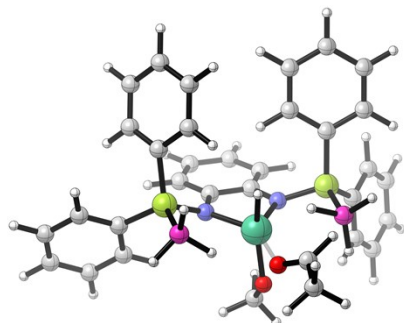
L



Ti	7.492213000	0.703461000	29.571988000
H	8.035424000	1.233470000	31.111936000
P	9.073929000	3.353496000	30.125592000
P	4.507283000	0.254182000	29.554715000
N	7.705751000	2.730336000	29.316766000
N	5.646090000	1.342411000	28.979685000
C	6.616343000	3.479707000	28.847191000
C	5.439193000	2.688195000	28.661454000
C	4.232252000	3.272659000	28.235783000
H	3.337207000	2.646165000	28.111297000
C	4.178841000	4.653138000	27.980695000
H	3.235764000	5.111550000	27.647231000
C	5.330911000	5.439259000	28.156097000
H	5.295140000	6.521243000	27.957614000
C	6.539880000	4.867759000	28.587646000
H	7.417811000	5.505442000	28.731736000
C	9.624305000	4.849036000	29.200487000
C	10.008704000	4.674352000	27.854502000
H	9.947026000	3.675637000	27.396608000
C	10.456519000	5.768689000	27.101129000
H	10.746414000	5.624866000	26.049189000
C	10.537999000	7.043879000	27.687768000
H	10.890208000	7.902470000	27.095973000
C	10.169781000	7.218348000	29.031754000

H	10.233568000	8.214317000	29.496963000
C	9.712931000	6.126321000	29.787905000
H	9.406988000	6.271249000	30.834356000
C	8.466776000	3.983459000	31.737729000
C	9.400867000	4.351371000	32.728695000
H	10.477991000	4.253477000	32.523742000
C	8.955563000	4.824092000	33.974170000
H	9.688690000	5.107299000	34.744973000
C	7.579346000	4.927406000	34.238034000
H	7.231018000	5.300215000	35.213550000
C	6.648411000	4.546996000	33.255836000
H	5.568226000	4.623998000	33.455361000
C	7.086696000	4.070454000	32.011066000
H	6.355669000	3.763223000	31.250517000
C	3.404954000	-0.312752000	28.219215000
C	2.355560000	-1.215670000	28.494151000
H	2.167087000	-1.547228000	29.527359000
C	1.555671000	-1.694744000	27.445762000
H	0.734752000	-2.395873000	27.661144000
C	1.806624000	-1.284928000	26.124050000
H	1.177968000	-1.662936000	25.303672000
C	2.863485000	-0.400458000	25.849023000
H	3.064732000	-0.084787000	24.814113000
C	3.667251000	0.084172000	26.892903000
H	4.502181000	0.772343000	26.691235000
C	3.483945000	1.126779000	30.791705000
C	2.129750000	1.453514000	30.584681000
H	1.618251000	1.125426000	29.667813000
C	1.436380000	2.206854000	31.546051000
H	0.379652000	2.464557000	31.378811000
C	2.092161000	2.638808000	32.710195000
H	1.546511000	3.228823000	33.462651000
C	3.447187000	2.321789000	32.913129000
H	3.966181000	2.659525000	33.822642000
C	4.146133000	1.571264000	31.957721000
H	5.211435000	1.340512000	32.111010000
B	10.645135000	2.239311000	30.260162000
H	10.438725000	1.303374000	31.027396000
H	11.457931000	3.047667000	30.717579000
H	10.925102000	1.922580000	29.104808000
B	5.759209000	-1.033041000	30.232101000
H	6.368709000	-0.379540000	31.097853000
H	6.489054000	-1.202428000	29.234662000
H	5.326258000	-2.084293000	30.659878000
O	8.739368000	-0.820002000	30.504093000
C	9.931669000	-0.984195000	30.216420000
H	10.356020000	-0.446129000	29.337408000
C	10.821400000	-1.891688000	30.997912000
H	11.279757000	-2.643757000	30.320733000
H	11.660106000	-1.289953000	31.408904000
H	10.272469000	-2.389347000	31.818053000
O	8.568023000	0.361792000	28.138931000
C	8.730874000	1.001206000	26.902569000
H	9.809958000	1.027584000	26.627346000
H	8.183049000	0.458565000	26.098952000
H	8.352138000	2.047708000	26.936927000

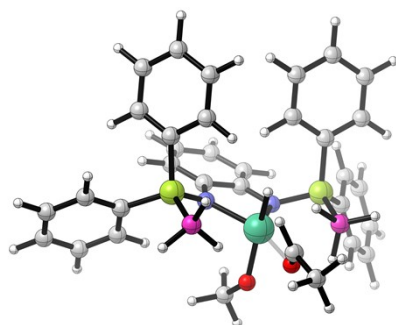
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Ti	7.990471000	0.874447000	29.641093000
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P	9.008167000	3.754138000	30.260221000
P	5.044852000	-0.055322000	29.527152000
N	7.818540000	2.906236000	29.426630000
N	6.071129000	1.179973000	28.999569000
C	6.650941000	3.458441000	28.880342000
C	5.642630000	2.475047000	28.661812000
C	4.377083000	2.867148000	28.185980000
H	3.591571000	2.118160000	28.024731000
C	4.122810000	4.223179000	27.911186000
H	3.132844000	4.522548000	27.535327000
C	5.122734000	5.188087000	28.112443000
H	4.921520000	6.247413000	27.891861000
C	6.387027000	4.812684000	28.601359000
H	7.161147000	5.571203000	28.773246000
C	9.654925000	5.111018000	29.212292000
C	10.288709000	4.715345000	28.014252000
H	10.395107000	3.643509000	27.785038000
C	10.769170000	5.683879000	27.121623000
H	11.255345000	5.369861000	26.185594000
C	10.629579000	7.050454000	27.422056000
H	11.008706000	7.809580000	26.721141000
C	10.002802000	7.446174000	28.615734000
H	9.887244000	8.515569000	28.850898000
C	9.510805000	6.480968000	29.509318000
H	9.000008000	6.795179000	30.431485000
C	8.222642000	4.508787000	31.727055000
C	8.980884000	5.310231000	32.607255000
H	10.036800000	5.530740000	32.384982000
C	8.393503000	5.811987000	33.779113000
H	8.987825000	6.434463000	34.465760000
C	7.053809000	5.509648000	34.080796000
H	6.595970000	5.904824000	35.000390000
C	6.305987000	4.692904000	33.216191000
H	5.261214000	4.439892000	33.449539000
C	6.887221000	4.185517000	32.044098000
H	6.306377000	3.528666000	31.380890000
C	3.886409000	-0.513327000	28.189544000
C	2.742182000	-1.291083000	28.465440000
H	2.497321000	-1.566760000	29.503091000
C	1.917810000	-1.720901000	27.413959000
H	1.021346000	-2.320551000	27.633966000
C	2.237830000	-1.389968000	26.085772000
H	1.589184000	-1.727973000	25.263438000
C	3.389542000	-0.633389000	25.808673000
H	3.646332000	-0.378280000	24.769185000
C	4.215650000	-0.198011000	26.856014000
H	5.119045000	0.396004000	26.651119000
C	4.061379000	0.698359000	30.876084000
C	2.742715000	1.170246000	30.725736000
H	2.197224000	1.000010000	29.786243000
C	2.123317000	1.865362000	31.778094000
H	1.094153000	2.235006000	31.655863000

C	2.818414000	2.096744000	32.976158000
H	2.330804000	2.642780000	33.798706000
C	4.138310000	1.632800000	33.124089000
H	4.689004000	1.814897000	34.059664000
C	4.761892000	0.936453000	32.079311000
H	5.809227000	0.599777000	32.170558000
B	10.227169000	2.343659000	30.668687000
H	9.350838000	1.500095000	31.004500000
H	10.873003000	2.573172000	31.682229000
H	10.861796000	2.056735000	29.667232000
B	6.247338000	-1.485871000	29.993248000
H	7.336395000	-1.060418000	29.557244000
H	5.977397000	-2.436183000	29.268353000
H	6.232200000	-1.707913000	31.191454000
O	9.503444000	-0.846105000	30.257928000
C	10.404261000	-0.927334000	31.082179000
H	10.685815000	-0.028629000	31.694126000
C	11.171945000	-2.188845000	31.328747000
H	12.255806000	-1.999858000	31.170044000
H	11.060925000	-2.480325000	32.395961000
H	10.820414000	-3.004422000	30.670632000
O	8.920089000	0.382425000	28.124903000
C	8.627358000	0.942205000	26.870440000
H	9.567857000	1.069830000	26.285339000
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H	8.129416000	1.938442000	26.940496000

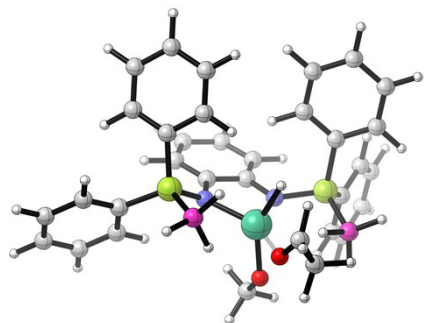
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P	5.170070000	-0.020331000	29.620634000
N	7.931769000	3.012911000	29.190834000
N	6.141622000	1.269864000	29.119431000
C	6.699914000	3.525869000	28.760944000
C	5.669694000	2.539085000	28.755438000
C	4.353363000	2.912106000	28.417279000
H	3.547363000	2.168302000	28.423893000
C	4.071302000	4.243648000	28.064979000
H	3.041517000	4.524032000	27.796623000
C	5.092732000	5.207308000	28.046584000
H	4.869854000	6.245024000	27.755825000
C	6.407388000	4.852759000	28.397009000
H	7.207231000	5.604213000	28.379473000
C	9.803626000	5.267059000	29.124574000
C	10.829141000	4.963011000	28.203754000
H	11.181939000	3.924607000	28.108481000
C	11.395714000	5.980450000	27.421067000
H	12.196585000	5.737392000	26.705934000
C	10.948291000	7.305703000	27.556837000
H	11.397298000	8.103964000	26.946500000
C	9.929550000	7.613189000	28.475512000

H	9.577285000	8.650506000	28.582992000
C	9.355902000	6.598830000	29.256833000
H	8.554787000	6.840708000	29.971708000
C	8.253918000	4.573521000	31.527540000
C	8.884928000	5.545053000	32.332934000
H	9.872412000	5.940408000	32.050844000
C	8.255203000	6.003860000	33.500436000
H	8.751088000	6.761426000	34.126659000
C	6.997729000	5.495367000	33.869855000
H	6.504055000	5.862182000	34.782601000
C	6.377080000	4.514437000	33.078503000
H	5.396324000	4.104118000	33.359331000
C	7.003802000	4.045678000	31.914674000
H	6.524977000	3.261516000	31.311477000
C	4.006855000	-0.458962000	28.279512000
C	2.926157000	-1.329248000	28.536249000
H	2.738111000	-1.690106000	29.559450000
C	2.096010000	-1.745477000	27.483949000
H	1.250594000	-2.419887000	27.690022000
C	2.348032000	-1.308909000	26.171593000
H	1.696505000	-1.637848000	25.347756000
C	3.436797000	-0.459317000	25.911930000
H	3.641234000	-0.120938000	24.884776000
C	4.267889000	-0.036398000	26.960805000
H	5.121221000	0.629732000	26.765686000
C	4.176080000	0.633930000	31.014904000
C	2.820882000	1.007160000	30.921810000
H	2.261492000	0.833108000	29.990735000
C	2.181342000	1.604740000	32.020793000
H	1.123622000	1.898416000	31.942530000
C	2.890843000	1.833975000	33.211000000
H	2.386812000	2.301836000	34.070844000
C	4.245672000	1.466455000	33.303462000
H	4.805177000	1.643597000	34.234924000
C	4.890238000	0.869173000	32.210684000
H	5.959787000	0.601695000	32.257703000
B	10.255503000	2.401443000	30.450948000
H	9.373040000	1.665590000	30.976156000
H	11.094416000	2.596180000	31.313941000
H	10.666997000	1.989238000	29.375086000
B	6.387865000	-1.459676000	30.016019000
H	7.439760000	-1.025479000	29.516529000
H	6.047767000	-2.427104000	29.344414000
H	6.447804000	-1.651720000	31.221879000
O	9.737931000	-0.548255000	30.156103000
C	9.661927000	-1.285536000	31.135402000
H	8.761110000	-1.217893000	31.799664000
C	10.721829000	-2.279369000	31.484350000
H	11.087189000	-2.077776000	32.514247000
H	10.270468000	-3.294823000	31.511458000
H	11.559931000	-2.247457000	30.764104000
O	8.734010000	0.296091000	27.939270000
C	8.265813000	0.710098000	26.684015000
H	9.110462000	0.740982000	25.957614000
H	7.510086000	-0.010393000	26.290040000
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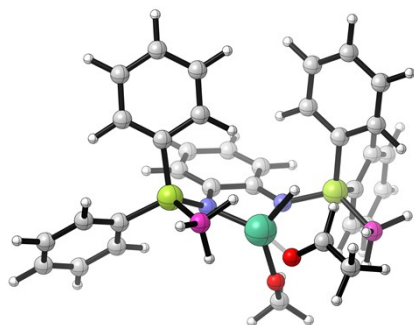
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P	5.033729000	-0.026645000	29.525907000
N	7.884350000	2.872546000	29.284568000
N	6.061554000	1.192656000	28.976200000
C	6.687245000	3.456599000	28.843399000
C	5.645451000	2.499042000	28.672133000
C	4.360630000	2.909574000	28.273013000
H	3.557711000	2.169667000	28.151563000
C	4.107119000	4.271841000	28.032942000
H	3.102288000	4.590670000	27.717753000
C	5.132335000	5.217342000	28.195655000
H	4.934704000	6.283804000	28.008157000
C	6.418376000	4.819677000	28.602429000
H	7.204409000	5.570392000	28.742527000
C	9.579823000	5.192739000	29.077916000
C	9.969169000	4.993502000	27.736070000
H	10.002729000	3.972614000	27.326106000
C	10.296117000	6.092037000	26.929149000
H	10.592287000	5.930682000	25.881609000
C	10.249572000	7.394523000	27.457265000
H	10.509786000	8.255801000	26.823358000
C	9.870209000	7.594683000	28.794722000
H	9.830559000	8.612956000	29.211502000
C	9.531434000	6.498684000	29.604899000
H	9.212462000	6.660467000	30.644978000
C	8.522124000	4.300603000	31.652377000
C	9.429794000	4.855533000	32.579229000
H	10.498800000	4.928528000	32.324260000
C	8.974224000	5.298600000	33.831377000
H	9.686909000	5.727611000	34.552346000
C	7.613825000	5.182818000	34.165989000
H	7.256814000	5.530722000	35.147368000
C	6.712989000	4.613180000	33.249710000
H	5.647626000	4.512474000	33.507415000
C	7.162391000	4.165407000	31.997932000
H	6.456908000	3.707903000	31.291371000
C	3.955602000	-0.597088000	28.169095000
C	2.936832000	-1.540602000	28.422328000
H	2.751692000	-1.892634000	29.449249000
C	2.167138000	-2.039778000	27.360711000
H	1.370229000	-2.772465000	27.561111000
C	2.420044000	-1.612558000	26.045144000
H	1.816711000	-2.007460000	25.213805000
C	3.449533000	-0.690632000	25.790548000
H	3.655678000	-0.363248000	24.760242000
C	4.220708000	-0.184327000	26.848298000
H	5.034622000	0.532196000	26.659930000
C	3.984699000	0.746531000	30.808937000
C	2.599796000	0.961809000	30.678433000
H	2.068098000	0.607376000	29.782942000
C	1.899324000	1.642051000	31.688656000
H	0.817174000	1.813460000	31.581884000

C	2.579447000	2.112524000	32.823493000
H	2.028305000	2.645862000	33.613553000
C	3.965767000	1.907577000	32.948024000
H	4.503855000	2.277778000	33.833869000
C	4.671910000	1.229154000	31.945388000
H	5.763844000	1.089579000	32.026564000
B	10.585172000	2.428411000	30.143287000
H	9.948378000	1.384581000	30.347825000
H	11.286963000	2.679648000	31.116939000
H	11.141039000	2.422092000	29.053790000
B	6.314067000	-1.316552000	30.128336000
H	7.198276000	-1.128324000	29.266545000
H	5.929070000	-2.469723000	30.011203000
H	6.648255000	-0.994184000	31.260440000
O	9.297792000	-0.850779000	30.346899000
C	9.598184000	-1.045802000	31.521707000
H	9.208710000	-0.337862000	32.300504000
C	10.466522000	-2.178201000	31.958109000
H	11.362524000	-1.766323000	32.470758000
H	9.924396000	-2.783527000	32.716309000
H	10.769880000	-2.807466000	31.101723000
O	9.008875000	0.411498000	28.079507000
C	8.826806000	0.981178000	26.812910000
H	9.645625000	1.707930000	26.598145000
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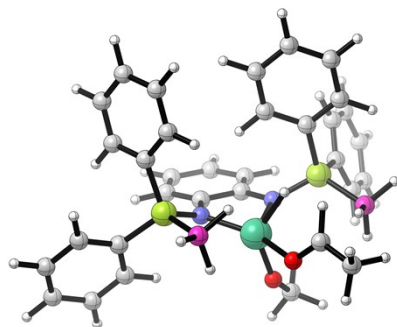
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N	7.706791000	2.836593000	29.664966000
N	5.856017000	1.259170000	29.040293000
C	6.558416000	3.498475000	29.210435000
C	5.497547000	2.601653000	28.869666000
C	4.241304000	3.084147000	28.459801000
H	3.430951000	2.374503000	28.237817000
C	4.025809000	4.467907000	28.351432000
H	3.043949000	4.846597000	28.030413000
C	5.069760000	5.358505000	28.655448000
H	4.910924000	6.444481000	28.567329000
C	6.323594000	4.888644000	29.081546000
H	7.111180000	5.607577000	29.329877000
C	9.298619000	5.191072000	30.060897000
C	9.794518000	5.332196000	28.747460000
H	9.924806000	4.439293000	28.118446000
C	10.109517000	6.602803000	28.246327000
H	10.488085000	6.706161000	27.218149000
C	9.946027000	7.741078000	29.055969000
H	10.194831000	8.738229000	28.661803000
C	9.469553000	7.602069000	30.369970000

H	9.344059000	8.489970000	31.008657000
C	9.145988000	6.331346000	30.874246000
H	8.759050000	6.226559000	31.898254000
C	8.179543000	3.743725000	32.319892000
C	8.997330000	3.631530000	33.462841000
H	10.064589000	3.394474000	33.339009000
C	8.446799000	3.810022000	34.743017000
H	9.089190000	3.715021000	35.632059000
C	7.081646000	4.106821000	34.889089000
H	6.652550000	4.254034000	35.892311000
C	6.264772000	4.218508000	33.749693000
H	5.196530000	4.463408000	33.856090000
C	6.806082000	4.032663000	32.468408000
H	6.160005000	4.114438000	31.583053000
C	3.861591000	-0.559849000	27.988977000
C	3.011356000	-1.681287000	28.100348000
H	2.895221000	-2.194930000	29.067961000
C	2.327747000	-2.153860000	26.969774000
H	1.665754000	-3.028830000	27.057198000
C	2.501171000	-1.520409000	25.726353000
H	1.967968000	-1.895654000	24.839789000
C	3.365480000	-0.418533000	25.611499000
H	3.511494000	0.069616000	24.636081000
C	4.050705000	0.061936000	26.738536000
H	4.739937000	0.915613000	26.655871000
C	3.668713000	0.630130000	30.696174000
C	2.267515000	0.543794000	30.596252000
H	1.803960000	0.063295000	29.721352000
C	1.461243000	1.087681000	31.610409000
H	0.365111000	1.020607000	31.530347000
C	2.050622000	1.720830000	32.716947000
H	1.416213000	2.147337000	33.509054000
C	3.450831000	1.818560000	32.808942000
H	3.919890000	2.320915000	33.668123000
C	4.262312000	1.279755000	31.802136000
H	5.359126000	1.379529000	31.863112000
B	10.645739000	2.602963000	30.695851000
H	10.572228000	1.500431000	31.230475000
H	11.304904000	3.406806000	31.361488000
H	11.009861000	2.573509000	29.524850000
B	6.173297000	-1.228426000	30.035501000
H	6.962991000	-1.199524000	29.071823000
H	5.831868000	-2.363190000	30.305465000
H	6.655668000	-0.627356000	31.013167000
O	9.117964000	-0.779271000	30.462546000
C	9.727335000	-0.727656000	31.533006000
H	9.405264000	0.013072000	32.306527000
C	10.875847000	-1.625419000	31.849437000
H	11.771333000	-0.989685000	32.019905000
H	10.684388000	-2.159115000	32.804723000
H	11.068132000	-2.341877000	31.030102000
O	8.940652000	0.756070000	28.356796000
C	9.281469000	1.557785000	27.264320000
H	10.388054000	1.641109000	27.180079000
H	8.889339000	1.121065000	26.317491000
H	8.856700000	2.581588000	27.380250000

TS_{No}



Ti	7.786478000	0.748697000	29.563077000
H	8.214002000	1.193720000	31.166154000
P	8.951814000	3.459015000	30.645629000
P	4.846445000	0.034632000	29.630630000
N	7.825521000	2.808071000	29.542620000
N	5.880666000	1.251827000	29.125260000
C	6.717365000	3.447902000	28.964760000
C	5.608171000	2.566011000	28.737351000
C	4.406423000	3.039085000	28.178311000
H	3.577870000	2.338701000	28.001844000
C	4.283998000	4.394459000	27.831477000
H	3.345395000	4.765723000	27.393094000
C	5.371004000	5.263431000	28.030050000
H	5.289422000	6.322066000	27.739841000
C	6.577448000	4.802760000	28.583999000
H	7.410450000	5.499875000	28.714326000
C	9.242695000	5.222189000	30.183948000
C	10.053952000	5.485125000	29.058505000
H	10.514744000	4.646879000	28.515439000
C	10.264078000	6.804651000	28.632721000
H	10.887521000	7.001097000	27.746901000
C	9.681607000	7.874479000	29.335550000
H	9.847087000	8.909876000	29.000044000
C	8.893350000	7.618869000	30.469752000
H	8.440529000	8.452849000	31.027224000
C	8.672060000	6.298199000	30.893252000
H	8.038792000	6.101651000	31.770339000
C	8.076584000	3.601503000	32.253120000
C	8.811483000	3.917020000	33.413776000
H	9.903061000	4.044604000	33.346978000
C	8.149236000	4.065884000	34.643449000
H	8.725412000	4.310755000	35.549113000
C	6.754883000	3.904606000	34.716738000
H	6.236167000	4.029862000	35.680141000
C	6.024304000	3.581029000	33.559650000
H	4.933526000	3.445151000	33.609286000
C	6.681503000	3.420923000	32.330628000
H	6.115177000	3.146496000	31.429468000
C	3.801179000	-0.511135000	28.238639000
C	2.634735000	-1.274625000	28.451214000
H	2.302106000	-1.503685000	29.475570000
C	1.895705000	-1.737585000	27.351800000
H	0.980488000	-2.325945000	27.517539000
C	2.321784000	-1.448264000	26.043575000
H	1.738171000	-1.810289000	25.183725000
C	3.491749000	-0.698285000	25.832777000
H	3.826638000	-0.472350000	24.809095000
C	4.235061000	-0.230322000	26.926883000
H	5.151656000	0.360735000	26.778063000
C	3.731476000	0.673151000	30.923685000
C	2.504307000	1.299566000	30.618335000
H	2.148424000	1.337488000	29.578423000
C	1.731520000	1.863618000	31.644736000
H	0.775999000	2.351820000	31.401817000

C	2.175106000	1.802218000	32.976912000
H	1.563227000	2.239842000	33.780197000
C	3.398277000	1.180711000	33.283561000
H	3.748053000	1.128627000	34.325663000
C	4.180378000	0.623376000	32.261202000
H	5.145463000	0.151960000	32.496733000
B	10.706515000	2.645131000	30.704094000
H	10.648119000	1.510967000	31.169688000
H	11.327909000	3.422258000	31.432931000
H	11.113642000	2.674782000	29.543925000
B	6.209579000	-1.199318000	30.193547000
H	6.891033000	-1.286210000	29.157109000
H	5.852587000	-2.290263000	30.594694000
H	6.820178000	-0.548379000	31.061527000
O	9.251918000	-0.758114000	30.207329000
C	9.885440000	-0.761793000	31.267161000
H	9.562559000	-0.084800000	32.095678000
C	11.061264000	-1.649090000	31.496215000
H	11.941258000	-1.005572000	31.711493000
H	10.893501000	-2.264471000	32.405949000
H	11.262343000	-2.291447000	30.619457000
O	8.758476000	0.759841000	28.052532000
C	9.393254000	1.616003000	27.152084000
H	10.498624000	1.491489000	27.199453000
H	9.059270000	1.398770000	26.111626000
H	9.148435000	2.676258000	27.392722000

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